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Best Hermitian interpolation in presence of uncertainties

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Abstract: In PDE-constrained optimization, iterative algorithms are commonly efficiently accelerated by techniques relying on approximate evaluations of the functional to be minimized by an economical, but lower-fidelity model ("metamodel"). Various types of metamodels exist (interpolation polynomials, neural networks, Kriging models, etc). Such metamodels are constructed by precalculation of a database of functional values by the costly high-fidelity model. In adjoint-based numerical methods, derivatives of the functional are also available at the same cost, although usually with poorer accuracy. Thus, a question arises : should the derivative information, known to be less accurate, be used to construct the metamodel or ignored ? As a first step to answer this question, we consider the case of the Hermitian interpolation of a function of a single variable, when the function values are known exactly, and the derivatives only approximately, assuming a uniform upper bound ϵ on this approximation is known. The classical notion of best approximation is revisited in this context, and a criterion is introduced to define the best set of interpolation points. This set is identified by either analytical or numerical means. If $n+1$ is the number of interpolation points, it is advantageous to account for the derivative information when $\epsilon \leq \epsilon_0$, where ϵ_0 decreases with n, and this is in favor of piecewise, low-degree Hermitian interpolants. In all our numerical tests, we have found that the distribution of Chebyshev points is always close to optimal, and provides bounded approximants with close-to-least sensitivity to the uncertainties.

Key-words: Hermitian interpolation, interpolation error, uncertainties, best approximant, Chebyshev interpolation points

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Meilleure approximation hermitienne en présence d'incertitudes

Résumé : En optimisation distribuée (sous contrainte d'équations aux dérivées partielles), il est courant d'accélérer les algorithmes itératifs par des techniques s'appuyant sur des évaluations approchées de la fonctionnelle à minimiser par un modèle économique de basse fidélité ("métamodèle"). Différent types de métamodèles sont possibles (polynômes d'interpolation, réseaux de neurones, modèles de krigeage, etc). Ces métamodèles sont construits à partir d'une base de données de valeurs de fonctionnelle précalculées par le modèle coûteux de haute fidélité. Dans le cas de méthodes numériques avec équation adjointe, on dispose également au même coût des valeurs de dérivée de fonctionnelle, même si, en général, ces valeurs sont connues avec une moindre précision. Ce contexte soulève alors la question suivante : l'information sur les dérivées, connue pour être moins précise, doit-elle être prise en compte dans la construction du métamodèle ? Comme première étape pour aborder cette question, on considère le cas d'un métamodèle par interpolation polynômiale, de Lagrange ou hermitienne, lorsque les valeurs interpolées de la fonction sont connues exactement, et celles de la dérivée seulement approximativement, en supposant qu'une borne supérieure uniforme est connue sur cette approximation. Ceci nous permet de revisiter la notion classique de meilleure approximation, et d'introduire un critère nous permettant de définir le choix optimal des points d'interpolation. Ce choix est identifié par voie analytique ou numérique. Si les points d'interpolation sont en nombre $n + 1$, il est avantageux de prendre en compte l'information sur les dérivées dès lors que $\epsilon \leq \epsilon_0$, où ϵ_0 décroit avec n, ce qui milite en faveur d'interpolants hermitiens de faible degré par morceaux. Dans tous nos tests numériques, on a constaté que la distribution de points de Tchebyshev est toujours proche de l'optimalité, et fournit des approximants bornés de sensibilté quasi-minimale aux incertitudes.

Mots-clés : Interpolation hermitienne, erreur d'interpolation, incertitudes, meilleur approximant, points d'interpolation de Tchebysheff

1 Introduction : the classical notion of best approximation

Let n be an integer and x_0 , x_1 , ... , x_n be $n+1$ distinct points of the normalized interval [-1,1]. Let $\pi(x)$ be the following polynomial of degree $n+1$:

$$\boxed{\pi(x) = \prod_{i=0}^{n} (x - x_i)} \tag{1}$$

and consider the following $n+1$ polynomials of degree n :

$$\mathsf{L}_i(x) = \prod_{\substack{j = 0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \qquad (i = 0, 1, ..., n) \tag{2}$$

Clearly :

$$\forall i, j \in \{0, 1, ..., n\} \ : \ \mathsf{L}_i(x_j) = \delta_{i,j} \tag{3}$$

where δ stands for the Krönecker's symbol. Application of L'Hospital's rule yields the following compact formula :

$$\mathsf{L}_i(x) = \frac{\pi(x)}{\pi'(x_i)(x - x_i)} \tag{4}$$

Let $f \ : \ [-1, 1] \longrightarrow \mathbb{R}$ be a smooth function of the real variable x. The polynomial

$$\boxed{P_n(x) = \sum_{i=0}^{n} f(x_i)\, \mathsf{L}_i(x)} \tag{5}$$

is of degree at most equal to n, and it clearly satisfies the following interpolation conditions:

$$\forall i \in \{0, 1, ..., n\} \ : \ P_n(x_i) = f(x_i) \tag{6}$$

One such interpolant is unique among all polynomials of degree $\leq n$. Thus, $P_n(x)$ is the Lagrange interpolation polynomial of f at the points $\{x_i\}_{(0 \leq i \leq n)}$.

It is well-known that if $f \in \mathsf{C}^{n+1}\big([-1, 1]\big)$, for any given $x \in [a, b]$, the interpolation error is given by :

$$\boxed{e_n(x) = f(x) - P_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\, \pi(x)} \tag{7}$$

for some $\xi \in [-1, 1]$.

Proof : Let $x \in [-1, 1]$ be given. If $x = x_i$ for some i, the result is trivially satisfied. Otherwise, $\pi(x) \neq 0$; then let

$$\lambda = \frac{e_n(x)}{\pi(x)}$$

so that

$$f(x) = P_n(x) + \lambda \pi(x)$$

and define the function

$$\phi(t) = f(t) - P_n(t) - \lambda \pi(t) \qquad (t \in [-1, 1])$$

The function $\phi(t)$ is of class $\mathsf{C}^{n+1}\big([-1,1]\big)$ and it admits a nonempty set of roots in the interval [-1,1] that includes $X = \{x_0\,,\ x_1\,,\ ...\,,\ x_n\,,\ x\}$. The $n+2$ elements of X are distinct and can be arranged as the elements of a strictly increasing sequence $\{x_i^0\}_{(0\le i\le n+1)}$ whose precise definition depends on the position of x w.r.t. the interpolation points $\{x_i\}_{(0\le i\le n)}$. By application of Rolle's theorem to $\phi(t) = \phi^{(0)}(t)$ over the subinterval $[x_i^0, x_{i+1}^0]$ $(i = 0, 1, ..., n)$, it follows that $\phi'(t)$ admits a root x_i^1 in the open interval $]x_i^0, x_{i+1}^0[$, and this, for each i. In this way we identify a strictly-increasing sequence of $n+1$ roots of $\phi'(t)$, $\{x_i^1\}_{(0\le i\le n)}$. Then Rolle's theorem can be applied in a similar way, this time to $\phi'(t)$, and so on to the successive derivatives of $\phi(t)$. We conclude that in general $\phi^{(k)}(t)$ admits at least $n+2-k$ distinct roots in [-1,1], $\{x_i^k\}_{0\le i\le n+1-k}$ $(0 \le k \le n+1)$. In particular, for $k = n+1$, $\phi^{(n+1)}(t)$ admits at least one root, x_0^{n+1}, hereafter denoted ξ for simplicity. But since $P_n^{(n+1)}(\xi) = 0$ and $\pi^{(n+1)}(\xi) = (n+1)!$, one gets :

$$\lambda = \frac{f^{(n+1)}(\xi)}{(n+1)!}$$

and the conclusion follows. □

Hence, if

$$K = \frac{1}{(n+1)!} \max_{x\in[-1,1]} \left|f^{(n+1)}(x)\right| \tag{8}$$

we have :

$$\forall x \in [-1,1]\,,\ |e_n(x)| \le K\,|\pi(x)| \tag{9}$$

Therefore, a natural way to optimize the choice of interpolation points *a priori*, that is, independently of f, is to solve the following classical min-max problem :

$$\boxed{\min_{\substack{\{x_i\}_{(0\le i\le n)} \\ x_i \in [-1,1]\,,\ \forall i}} \ \max_{x\in[-1,1]} |\pi(x)|} \tag{10}$$

In view of this, the problem is to find among all polynomials $\pi(x)$ whose highest-degree term is precisely x^{n+1}, and that admit $n+1$ distinct roots in the interval [-1,1], an element, unique or not, that minimizes the sup-norm over [-1,1].

The solution of this problem is given by the $n+1$ roots of the Chebyshev polynomial of degree $n+1$. Before proving this, let us establish a few auxiliary results. Let k be an arbitrary integer and $T_k(x)$ denote the Chebyshev polynomial of degree k. Recall that for $x \in [-1,1]$:

$$T_k(x) = \cos\!\big(k \cos^{-1} x\big) \qquad (k \in \mathbb{N}) \tag{11}$$

so that, for $k \ge 1$ and $x \in [-1,1]$:

$$T_{k+1}(x) + T_{k-1}(x) = \cos\!\big(\overline{k+1}\theta\big) + \cos\!\big(\overline{k-1}\theta\big) = 2\cos(k\theta)\,\cos\theta = 2xT_k(x) \tag{12}$$

where one has let

$$x = \cos\theta \qquad (0 \le \theta \le \pi) \tag{13}$$

Thus, if the leading term in $T_k(x)$ is say $a_k x^k$, the following recursion applies :

$$a_{k+1} = 2a_k \qquad (k \ge 1) \tag{14}$$

and since $a_0 = a_1 = 1$, it follows that :

$$a_k = 2^{k-1} \qquad (k \ge 1) \tag{15}$$

Therefore, an admissible candidate solution for the min-max problem, (10), is the polynomial

$$\boxed{\pi^*(x) = \frac{1}{2^n}\, T_{n+1}(x)} \tag{16}$$

It remains to establish that $\pi^*(x)$ is the best choice among all admissible polynomials, and its roots the best possible interpolation points. To arrive at this, we claim the following :

Lemma 1
For all admissible polynomial $q(x)$ one has :

$$\|\pi^*\| \leq \left\|q\right\| \tag{17}$$

where $\|\ \|$ is the sup-norm over [-1,1].

Proof : Assume otherwise that an admissible polynomial $q(x)$ of strictly smaller sup-norm over [-1,1] exists :

$$\left\|q\right\| < \|\pi^*\| \tag{18}$$

Let $r(x) = \pi^*(x) - q(x)$. Since the admissible polynomials $\pi^*(x)$ and $q(x)$ have the same leading term, x^{n+1}, the polynomial $r(x)$ is of degree at most n. Let us examine the sign of this polynomial at the $n+2$ points

$$\eta_i = \cos\frac{i\pi}{n+1} \qquad i = 0, 1, ..., n+1, \tag{19}$$

at which $\pi^*(x)$ as well as $T_{n+1}(x)$ achieves a local extremum. At such a point,

$$\left|\pi^*(\eta_i)\right| = \frac{1}{2^n} = \|\pi^*\| > \left\|q\right\| = \max_{x\in[-1,1]} \left|q(x)\right| \geq \left|q(\eta_i)\right| \tag{20}$$

and $r(\eta_i)$ is nonzero and has the sign of the strictly-dominant term $\pi^*(\eta_i) = \frac{1}{2^n}\, T_{n+1}(\eta_i) = \frac{(-1)^i}{2^n}$. Therefore, $r(x)$ admits at least $n+1$ sign alternations and as many distinct roots. But this is in contradiction with the degree of this polynomial. The contradiction is removed by rejecting the assumption made on $\left\|q\right\|$. □

Consequently, in (10), the min-max is achieved by the roots of $T_{n+1}(x)$:

$$\boxed{x_i^* = \cos\frac{(2i+1)\pi}{2(n+1)} \qquad (i = 0, 1, ..., n)} \tag{21}$$

and the value of the min-max is $\frac{1}{2^n}$.

2 Best Hermitian approximation

Now assume that the points $\{x_i\}_{(0\leq i\leq n)}$ are used as a support to interpolate the function values $\{y_i = f(x_i)\}_{(0\leq i\leq n)}$, but also the derivatives $\{y_i' = f'(x_i)\}_{(0\leq i\leq n)}$, that is a set of $2(n+1)$ data. Thus, we anticipate that the polynomial of least degree complying with these interpolation conditions, say $H_{2n+1}(x)$, is of degree at most equal to $2n+1$. One such polynomial is necessarily of the form :

$$\boxed{H_{2n+1}(x) = P_n(x) + \pi(x)\,.\,Q(x)} \tag{22}$$

where the quotient $Q(x)$ should be adjusted to comply with the interpolation conditions on the derivatives. These conditions are :

$$y'_i = H'_{2n+1}(x_i) = P'_n(x_i) + \pi'_i \, . \, Q(x_i) \qquad (i = 0, 1, ..., n) \tag{23}$$

where

$$\pi'_i = \pi'(x_i) = \prod_{\substack{j=0 \\ j \neq i}} \left(x_i - x_j\right) \neq 0 \tag{24}$$

and since $\pi(x_i) = 0$. Thus $Q(x)$ is solely constrained by the following $n+1$ interpolation conditions :

$$Q_i = Q(x_i) = \frac{y'_i - P'_n(x_i)}{\pi'_i} \qquad (i = 0, 1, ..., n) \tag{25}$$

Therefore, the solution of least degree is obtained when $Q(x)$ is the Lagrange interpolation polynomial associated with the above function values :

$$Q(x) = \sum_{i=0}^{n} Q_i \, \mathsf{L}_i(x) \tag{26}$$

The corresponding solution is thus unique, and we will refer to it as the global Hermitian interpolant.

The interpolation error associated with the above global Hermitian interpolant $H_{2n+1}(x)$ is given by the following result valid when $f \in \mathsf{C}^{2n+2}\big([-1,1]\big)$:

$$\boxed{\forall x \in [-1,1]\,,\ \exists \eta \in [-1,1] \,/\, f(x) = H_{2n+1}(x) + \frac{f^{(2n+2)}(\eta)}{(2n+2)!}\,\pi^2(x)} \tag{27}$$

Proof : Let $x \in [-1,1]$ be given. If $x = x_i$ for some i, the result is trivially satisfied. Otherwise, $\pi(x) \neq 0$; then let

$$\mu = \frac{f(x) - H_{2n+1}(x)}{\pi^2(x)}$$

so that

$$f(x) = H_{2n+1}(x) + \mu\pi^2(x)$$

Let

$$\psi(t) = f(t) - H_{2n+1}(t) - \mu\pi^2(t) \qquad (t \in [-1,1])$$

The function $\psi(t)$ is of class $\mathsf{C}^{2n+2}\big([-1,1]\big)$, and similarly to the former function $\phi(t)$, it admits a nonempty set of roots in the interval [-1,1] that includes $X = \{x_0\,,\ x_1\,,\ \dots\,,\ x_n\,,\ x\} = \{x_i^0\}_{(0\leq i\leq n+1)}$. Hence, Rolle's theorem implies that in the open interval $]x_i, x_{i+1}[$ $(0 \leq i \leq n)$, a root x'_i of $\psi'(t)$ exists. But the interpolation points, at which the derivative also is fitted, are themselves $n+1$ other distinct roots of $\psi'(t)$. Thus we get a total of at least $2n+2$ roots for $\psi'(t)$, and by induction, $2n+1$ for $\psi''(t)$, and so on, and finally one, say η, for $\psi^{(2n+2)}(t)$. Now, since $H_{2n+1}^{(2n+2)}(\eta) = 0$ because the interpolant is of degree $2n+1$ at most, and since $\left(\pi^2(t)\right)^{(2n+2)}(t) = (2n+2)!$, one gets :

$$0 = f^{(2n+2)}(\eta) - 0 - \mu\,(2n+2)!$$

which yields the final result. □

As a consequence of (27), the formulation of the best approximation problem for the global Hermitian interpolant is as follows :

$$\boxed{\min_{\substack{\{x_i\}_{(0\le i\le n)}\\ x_i\in[-1,1],\ \forall i}} \ \max_{x\in[-1,1]} \pi^2(x)} \tag{28}$$

But, if we define the following functions of $\mathbb{R}^{n+1} \longrightarrow \mathbb{R}$:

$$\begin{cases} P(x_0,x_1,...,x_n) = \max\limits_{x\in[-1,1]} \pi^2(x) \\ p(x_0,x_1,...,x_n) = \max\limits_{x\in[-1,1]} |\pi(x)| \end{cases} \tag{29}$$

it is obvious that :

$$\forall x_0\,,\ x_1\,,\ ...\,,\ x_n\ :\ P(x_0,x_1,...,x_n) = p^2(x_0,x_1,...,x_n) \tag{30}$$

Hence the functions P and p achieve their minimums for the same sequence of interpolation points, and

$$\min_{\substack{\{x_i\}_{(0\le i\le n)}\\ x_i\in[-1,1],\ \forall i}} P(x_0,x_1,...,x_n) = \left(\min_{\substack{\{x_i\}_{(0\le i\le n)}\\ x_i\in[-1,1],\ \forall i}} p(x_0,x_1,...,x_n)\right)^2 = \frac{1}{4^n} \tag{31}$$

Therefore the best Hermitian interpolation is achieved for the same set of interpolation points as the best Lagrangian interpolation, that is, the roots, $\{x_i^*\}_{(0\le i\le n)}$ of (21), of the Chebyshev polynomial $T_{n+1}(x)$.

3 Best inexact Hermitian approximation

Now, we consider a new problem in which we assume that the function values $\{y_i\}_{(0\le i\le n)}$ are known, whereas only approximations $\{\bar{y}'_i\}_{(0\le i\le n)}$ of the derivatives $\{y'_i\}_{(0\le i\le n)}$ are available, and we let :

$$\delta y'_i = \bar{y}'_i - y'_i := \epsilon_i \qquad (i = 0,1,...,n) \tag{32}$$

Hence the computed interpolant is $\overline{H}_{2n+1}(x)$ instead of $H_{2n+1}(x)$, and in view of the definitions (22)-(25), we have :

$$\begin{cases} \delta H_{2n+1}(x) = \overline{H}_{2n+1}(x) - H_{2n+1}(x) = \pi(x)\,\delta Q(x) \\ \delta Q(x) = \sum\limits_{i=0}^{n} \delta Q_i\, \mathsf{L}_i(x) \\ \delta Q_i = \dfrac{\delta y'_i}{\pi'_i} = \dfrac{\epsilon_i}{\pi'_i} \end{cases} \tag{33}$$

Now, suppose an upper bound ϵ on the errors ϵ_i's is known :

$$|\epsilon_i| \le \epsilon \qquad (0 \le i \le n) \tag{34}$$

The following questions arise :

1. What is the corresponding upper bound on $\max_{x\in[-1,1]} |\delta H_{2n+1}(x)|$?
2. Can we choose the sequence of interpolation points $\{x_i\}_{(0\le i\le n)}$ to minimize this upper bound ?

3. Is the known sequence of the Chebyshev points a good approximation of the optimum sequence for this new problem ?

This report brings answers to these questions. Before this, let us motivate further the interest for this problem.

In practice, the problem is intended to model a situation of functional optimization in which the function f is a criterion to be optimized that depends on the design variable x through the numerical integration of a PDE and the derivative $f'(x)$ is computed by means of an adjoint equation. A database of function values and derivatives is compiled by Design of Experiment, and a surrogate model, or metamodel is constructed from it. This metamodel is then used in some way in the numerical optimization algorithm with the objective of improving computational efficiency. The success of such a strategy depends on the accuracy of the metamodel to represent the actual $f(x)$. If all the data were exact, and properly used, the accuracy would undoubtedly improve by the additional derivative information. However, in practice, in discrete PDE applications, the derivatives are almost inevitably computed with inferior accuracy. Therefore it is not clear that accounting for the derivatives is definitely advantageous if the accuracy of the data is poor. Should special precautions be taken to guarantee it ?

In this report, we try to identify how the interpolation points should be defined to minimize or reduce the effect on the metamodel accuracy of uncertainties on the derivatives only. It follows from (33) that :

$$\delta H_{2n+1}(x) = \pi(x) \sum_{i=0}^{n} \frac{\epsilon_i}{\pi'_i} \mathsf{L}_i(x) \tag{35}$$

which, by virtue of (4) simplifies as follows :

$$\delta H_{2n+1}(x) = \pi^2(x) \sum_{i=0}^{n} \frac{\epsilon_i}{\pi_i'^2 \, (x - x_i)} \tag{36}$$

Thus if (34) holds, we have :

$$|\delta H_{2n+1}(x)| \leq \epsilon \Delta(x) \tag{37}$$

where :

$$\boxed{\Delta(x) = \pi^2(x) \sum_{i=0}^{n} \frac{1}{\pi_i'^2 \, |x - x_i|}} \tag{38}$$

These considerations have lead us to analyze the min-max problem applied to the new criterion $\Delta(x)$ in place of $\pi^2(x)$. In summary, the solution of the min-max problem associated with the criterion $\Delta(x)$ minimizes the effect of uncertainties in the derivatives on the identification of the global Hermitian interpolant. In the subsequent sections, this solution is identified formally, or numerically, and compared with the Chebyshev distribution of points, which is optimal w.r.t. interpolation error. Lastly, the corresponding interpolants are compared by numerical experiment.

4 Formal or numerical treatment of the min-max-Δ problem

4.1 Notations and generalities

We wish to compare three particular relevant distributions of interpolation points in terms of performance w.r.t. the criterion $\Delta(x)$. These three distributions are symmetrical w.r.t. 0, and recall that the total number of interpolation points is $n + 1$. Thus, we let:

$$\boxed{n + 1 = 2m + \alpha} \tag{39}$$

and when n is odd ($\alpha = 0$; $n = 2m - 1 \geq 1$),

$$\{x_i\}_{0 \leq i \leq n} = \{\pm\xi_1, \pm\xi_2, ..., \pm\xi_m\} \tag{40}$$

where :

$$0 < \xi_1 < \xi_2 < ... < \xi_m \tag{41}$$

and $m \geq 1$. Otherwise, when n is even ($\alpha = 1$; $n = 2m \geq 0$), we adjoin to the list $\xi_0 = 0$ (once). We consider specifically :

1. The uniform distribution :
   - $n = 2m$: $\xi_0^u = 0$ associated with the interpolation point $x_0 = \xi_0 = 0$, and $\xi_k^u = \frac{k}{m}$ ($1 \leq k \leq m$) associated with 2 interpolation points $\pm\xi_k^u$.
   - $n = 2m - 1$: $\xi_k^u = \frac{2k-1}{n}$ ($1 \leq k \leq m$)
2. The Chebyshev distribution :
$$\xi_k^* = x_{m-k}^* = \cos\left(\frac{2(m-k)+1}{n+1}\,\frac{\pi}{2}\right) \qquad (1 \leq k \leq m) \tag{42}$$
3. The optimal distribution :
$$\bar{\xi} = \mathrm{Argmin}_{\xi} \max_{x \in [0,1]} \Delta(x;\xi) \tag{43}$$
   where $\xi = (\xi_1, \xi_2, ..., \xi_m)$ denotes the vector of adjustable parameters defining, along with $\xi_0 = 0$ if n is even, the distribution of interpolation points, and the dependence of the criterion Δ on ξ is here indicated explicitly for clarity. (Note that due to symmetry, the interval for x has been reduced to [0,1] without incidence on the result.)

To these three distributions are associated the corresponding values of the maximum of $\Delta(x;\xi)$ over $x \in [0,1]$; these maximums are denoted Δ^u, Δ^* and $\bar{\Delta}$ respectively.

As a result of these definitions, the polynomial $\pi(x)$ is expressed as follows :

$$\boxed{\pi(x) = x^{\alpha} \prod_{k=1}^{m} \left(x^2 - \xi_k^2\right) \qquad (n+1 = 2m+\alpha\,;\ \alpha = 0 \text{ or } 1)} \tag{44}$$

and for $x > 0$, the criterion $\Delta(x)$ becomes :

$$\Delta(x) = \pi^2(x) \sum_{i=0}^{n} \frac{1}{\pi_i'^2\,|x - x_i|} = \pi^2(x)\left[\frac{\alpha}{\pi_0'^2}\frac{1}{x} + \sum_{k=1}^{m} \frac{1}{\pi_k'^2}\left(\frac{1}{x+\xi_k} + \frac{1}{|x-\xi_k|}\right)\right] \tag{45}$$

Then, given x, let j be the index for which :

$$\boxed{\xi_{j-1} \leq x < \xi_j} \tag{46}$$

so that :

$$x - \xi_k \geq 0 \Longleftrightarrow k \leq j-1 \tag{47}$$

As a result :

$$\boxed{\Delta(x) = \pi^2(x)\left[\frac{\alpha}{\pi_0'^2}\frac{1}{x} + \sum_{k=1}^{j-1} \frac{1}{\pi_k'^2}\frac{2x}{x^2 - \xi_k^2} + \sum_{k=j}^{m} \frac{1}{\pi_k'^2}\frac{2\xi_k}{\xi_k^2 - x^2}\right]} \tag{48}$$

Calculation of the derivatives π'_k: First, for $\alpha = 0$, $\pi(x)$ is an even polynomial, and $\pi'_0 = 0$. Otherwise, for $\alpha = 1$,

$$\pi'_0 = \lim_{x\to 0} \frac{\pi(x)}{x} = \prod_{k=1}^{m} \left(-\xi_k^2\right) \qquad (\alpha = 1\,;\; n = 2m) \tag{49}$$

Regardless α, for $k \geq 1$:

$$\pi(x) = x^\alpha (x - \xi_k)(x + \xi_k) \prod_{\substack{i = 1 \\ i \neq k}} \left(x^2 - \xi_i^2\right) \tag{50}$$

so that :

$$\pi'_k = \lim_{x\to \xi_k} \frac{\pi(x)}{x - \xi_k} = 2\xi_k^{\alpha+1} \prod_{\substack{i = 1 \\ i \neq k}} \left(\xi_k^2 - \xi_i^2\right) \tag{51}$$

4.2 The particular case : $n + 1$ even ($\alpha = 0\,;\; n + 1 = 2m$)

Suppose that $0 < x < \xi_1$. Then $j = 1$ and (48) reduces to :

$$\Delta(x) = \pi^2(x) \sum_{k=1}^{m} \frac{1}{{\pi'_k}^2} \frac{2\xi_k}{\xi_k^2 - x^2} \tag{52}$$

But,

$$\pi^2(x) = \prod_{i=1}^{m} \left(x^2 - \xi_i^2\right)^2 \tag{53}$$

so that :

$$\Delta(x) = \sum_{k=1}^{m} \frac{2\xi_k}{{\pi'_k}^2} \times \prod_{\substack{i = 1 \\ i \neq k}}^{m} \left(\xi_i^2 - x^2\right)^2 \times \left(\xi_k^2 - x^2\right) \tag{54}$$

All the terms in this sum are composed of three factors : a positive constant and two positive factors that are monotone decreasing as x varies from 0 to ξ_1. Hence $\Delta(x)$ is monotone decreasing and :

$$\delta_0 = \max_{x\in[0,\xi_1]} \Delta(x) = \Delta(0) = \sum_{k=1}^{m} \frac{2\xi_k^3}{{\pi'_k}^2} \prod_{\substack{i = 1 \\ i \neq k}}^{m} \xi_i^4 = 2\left(\prod_{i=1}^{m} \xi_i^4\right) \sum_{k=1}^{m} \frac{1}{\xi_k {\pi'_k}^2} \qquad (\alpha = 0\,;\; n + 1 = 2m) \tag{55}$$

4.3 The particular case : $\xi_m < 1$

Suppose that $\xi_m < x < 1$. Then $j = m + 1$ and (48) reduces to :

$$\begin{aligned}\Delta(x) &= \pi^2(x) \left[\frac{\alpha}{{\pi'_0}^2} \frac{1}{x} + \sum_{k=1}^{m} \frac{1}{{\pi'_k}^2} \frac{2x}{x^2 - \xi_k^2} \right] \\ &= \frac{\alpha}{{\pi'_0}^2} x \prod_{i=1}^{m} \left(x^2 - \xi_i^2\right)^2 + \sum_{k=1}^{m} \frac{2}{{\pi'_k}^2} x^{2\alpha+1} \left(x^2 - \xi_k^2\right) \prod_{\substack{i = 1 \\ i \neq k}}^{m} \left(x^2 - \xi_i^2\right)^2\end{aligned} \tag{56}$$

All the terms in $\Delta(x)$ are products of positive factors that are monotone-increasing with x. Consequently, the maximum is achieved at $x = 1$. But :

$$\Delta(1) = \frac{\alpha}{\pi_0'^2} \prod_{i=1}^{m} \left(1 - \xi_i^2\right)^2 + \sum_{k=1}^{m} \frac{2}{\pi_k'^2} \left(1 - \xi_k^2\right) \prod_{\substack{i = 1 \\ i \neq k}}^{m} \left(1 - \xi_i^2\right)^2$$

This gives :

$$\delta_1 = \max_{x \in [\xi_m, 1]} \Delta(x) = \Delta(1) = \prod_{i=1}^{m} \left(1 - \xi_i^2\right)^2 \left[\frac{\alpha}{\pi_0'^2} + 2 \sum_{k=1}^{m} \frac{1}{\pi_k'^2 \left(1 - \xi_k^2\right)} \right] \tag{57}$$

4.4 Results

The min-max-Δ problem has been solved by either analytical or numerical means for values of n in the range from 0 to 40. The results are collected in Table 1 in which the first column indicates the number of interpolation points $n + 1$, the second gives the definition of the Chebyshev points ξ^* ($n \leq 4$), the third provides the definition of the optimal distribution $\bar{\xi}$, and the fourth a comparison of performance, by giving, when available the values of :

1. $\bar{\Delta} = \max_x \Delta(x, \bar{\xi})$, the upper bound on $\Delta(x)$ corresponding to the optimal distribution $\xi = \bar{\xi}$ of interpolation points;

2. $\bar{\Delta} = \max_x \Delta(x, \xi^*)$, the upper bound on $\Delta(x)$ corresponding to the approximately optimal distribution $\xi = \xi^*$ of interpolation points (Chebyshev distribution);

3. $\Delta^u = \max_x \Delta(x, \xi^u)$, the upper bound on $\Delta(x)$ corresponding to the uniform distribution $\xi = \xi^u$ of interpolation points.

The analytical results are related to the cases for which $n \leq 4$, and have been developed in Appendices A-E.

For $n + 1 \geq 10$, the distribution $\bar{\xi}$ (not given here) has been identified by a numerical minimization realized by a particle-swarm (PSO) algorithm. The table indicates the corresponding values of $\bar{\Delta}$.

From these results, one observes that the upper bound $\bar{\Delta}$ achieved when the distribution of interpolation points is optimized, is not only bounded, but it even diminishes with increasing n. The Chebyshev distribution has an almost equivalent performance. Inversely, the uniform distribution yields a value of the upper bound Δ^u that is unbounded with n. In conclusion, using the Chebyshev distribution, which is known explicitly, is highly recommended in practice.

number interpol. pts. : $n+1$ degree of interpolant : $2n+1$	Chebyshev points : ξ^*	$\bar{\xi} =$ $\text{Argmin}_{\xi}\text{max}_x \Delta$	Performance : $\bar{\Delta}$ Δ^* Δ^u
1 1	0	0	1 1 1
2 3	$\pm\frac{1}{\sqrt{2}} \doteq \pm 0.7071$	± 0.7549	0.3774 0.5 0.5
3 5	0 $\pm\frac{\sqrt{3}}{2} \doteq \pm 0.8660$	0 ± 0.8677	0.3258 0.3333 0.3755
4 7	$\pm\sqrt{\frac{1}{2}-\frac{1}{\sqrt{8}}} \doteq \pm 0.3827$ $\pm\sqrt{\frac{1}{2}+\frac{1}{\sqrt{8}}} \doteq \pm 0.9239$	± 0.351 ± 0.926	0.282 0.299 0.439
5 9	0 $\pm\sqrt{\frac{5-\sqrt{5}}{8}} \doteq \pm 0.5878$ $\pm\sqrt{\frac{5+\sqrt{5}}{8}} \doteq \pm 0.9511$	0 ± 0.571 ± 0.948	0.249 0.262 0.652
10 19			0.164 0.179 39.
11 21			0.154 0.167 111.
20 39			0.103 0.112 3.9×10^6
21 41			0.100 0.108 1.3×10^7

Table 1: Variation of the criterion $\max_x \Delta(x,\xi)$, related to Hermitian interpolation with uncertain derivatives, for different choices of the set $\xi = \{\xi_i\}$ $(i = 1,...,n)$ of interpolation points in [-1,1], and different degrees, $2n+1$; $\bar{\Delta} = \max_x \Delta(x,\bar{\xi})$, $\Delta^* = \max_x \Delta(x,\xi^*)$ and $\Delta^u = \max_x \Delta(x,\xi^u)$, where $\xi_i^u = -1 + \frac{2}{n-1}(i-1)$ $(i = 1,...,n)$.

5 Generalized Hermitian interpolation

5.1 Introduction and notations

In this section, we generalize the notions introduced in the first three to the situation where one wishes to construct a(the) low(est)-degree polynomial interpolant of the values, as well as the derivatives up to order, say p ($p \in \mathbb{N}$), of a given smooth function $f(x)$ over [-1,1]. The interpolation points are again denoted $\{x_i\}_{i=0,1,\dots,n}$, and we use the notation :

$$y_i^{(k)} = f^{(k)}(x_i) \qquad (k = 0, 1, \dots, p\,;\; i = 0, 1, \dots, n) \tag{58}$$

The interpolation polynomial is denoted $\mathsf{H}_{n,p}(x)$ and it is now constrained to the following $(p + 1)(n + 1)$ interpolation conditions :

$$\forall k \in \{0, 1, \dots, p\}\,,\; \forall i \in \{0, 1, \dots, n\} \;:\; \mathsf{H}_{n,p}^{(k)}(x_i) = y_i^{(k)} \tag{59}$$

We associate such kind of interpolation with the expression "generalized Hermitian interpolation".

5.2 Existence and uniqueness

We first establish existence and uniqueness by the following :

Theorem 1
There exists a unique polynomial $\mathsf{H}_{n,p}(x)$ *of degree at most equal to* $(p+1)(n+1)-1$ *satisfying the generalized interpolation conditions (59).*

Proof : by recurrence on p. For $p = 0$, the generalized Hermitian interpolation reduces to the classical Lagrange interpolation, whose solution is indeed unique among polynomials of degree at most equal to $(p + 1)(n + 1) - 1 = n$:

$$\mathsf{H}_{n,0}(x) = P_n(x) \tag{60}$$

For $p \geq 1$, assume $\mathsf{H}_{n,p-1}(x)$ exists and is unique among polynomials of degree at most equal to $p(n + 1) - 1$. This polynomial, by assumption, satisfies the following interpolation conditions :

$$\forall k \in \{0, 1, \dots, p-1\}\,,\; \forall i \in \{0, 1, \dots, n\} \;:\; \mathsf{H}_{n,p-1}^{(k)}(x_i) = y_i^{(k)} \tag{61}$$

Hence, by seeking $\mathsf{H}_{n,p}(x)$ in the form

$$\boxed{\mathsf{H}_{n,p}(x) = \mathsf{H}_{n,p-1}(x) + R(x)} \tag{62}$$

one finds that $R(x)$ should be of degree at most equal to $(p + 1)(n + 1) - 1$ and satisfy :

$$\forall k \in \{0, 1, \dots, p-1\}\,,\; \forall i \in \{0, 1, \dots, n\} \;:\; R^{(k)}(x_i) = 0 \tag{63}$$

and :

$$\forall i \in \{0, 1, \dots, n\} \;:\; R^{(p)}(x_i) = y_i^{(p)} - \mathsf{H}_{n,p-1}^{(p)}(x_i) \tag{64}$$

Now, (63) is equivalent to saying that $R(x)$ is of the form :

$$\boxed{R(x) = \prod_{i=0}^{n} (x - x_i)^p \,.\, Q(x) = \pi(x)^p\, Q(x)} \tag{65}$$

for some quotient $Q(x)$. Then, the derivative of order p of $R(x)$ at $x = x_i$ is calculated by Leibniz formula applied to the product $u(x)v(x)$ where :

$$u(x) = (x - x_i)^p \qquad v(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} (x - x_j)^p \,.\, Q(x) \tag{66}$$

This gives :

$$R^{(p)}(x_i) = \sum_{k=0}^{p} \binom{p}{k} u^{(k)}(x_i)\, v^{(p-k)}(x_i) \tag{67}$$

But, $u^{(k)}(x_i) = 0$ for all k except $k = p$ yielding :

$$R^{(p)}(x_i) = p!\, v(x_i) = p! \prod_{\substack{j=0 \\ j \neq i}}^{n} (x_i - x_j)^p\, Q(x_i) = p!\, \pi'(x_i)^p\, Q(x_i) \tag{68}$$

Thus, all the interpolation conditions are satisfied iff the polynomial $Q(x)$ fits the following interpolation conditions :

$$\boxed{\forall i \in \{0, 1, ..., n\} \;:\; Q(x_i) = Q_i = \frac{R^{(p)}(x_i)}{p!\pi'(x_i)^p} = \frac{y_i^{(p)} - \mathsf{H}_{n,p-1}^{(p)}(x_i)}{p!\pi'(x_i)^p}} \tag{69}$$

Therefore, solutions exist, and the lowest-degree solution is uniquely obtained when $Q(x)$ is the Lagrange interpolation polynomial associated with the above function values. This polynomial is of degree at most equal to n. Hence, $R(x)$ and $\mathsf{H}_{n,p}(x)$ are of degree at most equal to $p(n+1)+n = (p+1)(n+1)-1$. □

5.3 Interpolation error and best approximation

We have the following :

Theorem 2 (*Interpolation error associated with the generalized Hermitian interpolant)*
Assuming that $f \in \mathsf{C}^{(p+1)(n+1)}([-1,1])$, *we have:*

$$\boxed{\forall x \in [-1,1]\,,\ \exists \xi \in [-1,1] \;:\; f(x) = \mathsf{H}_{n,p}(x) + \pi(x)^{p+1} \frac{f^{([(p+1)(n+1)])}(\xi)}{[(p+1)(n+1)]!}} \tag{70}$$

Proof : Let $x \in [-1,1]$ be fixed. If $x = x_i$ for some $i \in \{0, 1, ..., n\}$, $f(x) = \mathsf{H}_{n,p}(x)$ and $\pi(x) = 0$, and the statement is trivial. Hence, assume now otherwise that $x \neq x_i$ for any $i \in \{0, 1, ..., n\}$. Then, define the constant :

$$\gamma = \frac{f(x) - \mathsf{H}_{n,p}(x)}{\pi(x)^{p+1}} \tag{71}$$

so that :

$$f(x) = \mathsf{H}_{n,p}(x) + \gamma\pi(x)^{p+1} \tag{72}$$

Using now the symbol t for the independent variable, one considers the function :

$$\theta(t) = f(t) - \mathsf{H}_{n,p}(t) - \gamma\pi(t)^{p+1} \tag{73}$$

By virtue of the interpolation conditions satisfied by the polynomial $\mathsf{H}_{n,p}(t)$:

$$\forall k \in \{0, 1, ..., p\}\,,\ \forall i \in \{0, 1, ..., n\}\ :\ \theta^{(k)}(x_i) = 0 \tag{74}$$

but additionally, by the choice of the constant γ, we also have :

$$\theta(x) = 0 \tag{75}$$

This makes $n+2$ distinct zeroes for $\theta(x)$: $x_0, x_1, ..., x_n$ and x. Thus, by application of Rolle's theorem in each of the $n+1$ consecutive intervals that these $n+2$ points once arranged in increasing order define, a zero of $\theta'(t)$ exists, yielding $n+1$ distinct zeroes for $\theta'(t)$, to which (74) adds $n+1$ distinct and different ones, for a total of $2(n+1) = 2n+2$ zeroes. Strictly between these, one finds $2(n+1)-1$ zeroes of $\theta''(t)$ to which (74) adds $n+1$ distinct and different ones, for a total of $3(n+1)-1 = 3n+2$ zeroes. Thus, for every new derivative, we find one less zero in every subinterval, but $n+1$ more by virtue of (74), for a total of n more, and this as long as (74) applies. Hence we get that $\theta^{(p)}(t)$ admits at least $(p+1)n+2$ distinct zeroes. For derivatives of higher order, the number of zeroes is one less for every new one; hence, $(p+1)n+1$ for $\theta^{(p+1)}(t)$, and so on. We finally get that $\theta^{([p+(p+1)n+1])}(t) = \theta^{([(p+1)(n+1)])}(t)$ admits at least one zero ξ, that is :

$$0 = f^{([(p+1)(n+1)])}(\xi) - \gamma[(p+1)(n+1)]! \tag{76}$$

because $\mathsf{H}^{([(p+1)(n+1)])}(\xi) = 0$ since the degree of $\mathsf{H}_{n,p}(t)$ is at most equal to $(p+1)(n+1)-1$, and the conclusion follows. $\square$

As a consequence of this result, it is clear that the best generalized Hermitian approximation is achieved by the Chebyshev distribution of interpolation points again.

5.4 Best inexact generalized Hermitian interpolation

Now suppose that all the data on f and its successive derivatives are exact, except for the derivatives of highest-order, $\{y_i^{(p)}\}$ that are subject to uncertainties $\{\epsilon_i\}_{i=0,1,...,n}$. Then, the uncertainties on the values $\{Q_i\}_{i=0,1,...,n}$ of the quotient $Q(x)$ are the following :

$$\delta Q_i = \frac{\epsilon_i}{p!\pi'(x_i)^p} \tag{77}$$

and on the quotient itself the following :

$$\delta Q(x) = \sum_{i=0}^{n} \frac{\epsilon_i}{p!\pi'(x_i)^p}\mathsf{L}_i(x) = \pi(x)\sum_{i=0}^{n} \frac{\epsilon_i}{p!\pi'(x_i)^{p+1}(x-x_i)} \tag{78}$$

and finally the uncertainty on the generalized Hermitian interpolant $\mathsf{H}_{n,p}(x)$ the following :

$$\delta\mathsf{H}_{n,p}(x) = \pi(x)^{p+1}\sum_{i=0}^{n} \frac{\epsilon_i}{p!\pi'(x_i)^{p+1}(x-x_i)} \tag{79}$$

In conclusion, for situations in which the uncertainties $\{\epsilon_i\}_{i=0,1,...,n}$ are bounded by the same number ϵ, the criterion that one should consider to conduct the min-max optimization of the interpolation points $\{x_i\}_{i=0,1,...,n}$ is now the following one to replace the former $\Delta(x)$:

$$\boxed{\Delta^{(p)}(x) = |\pi(x)|^{p+1}\sum_{i=0}^{n} \frac{1}{p!\,|\pi'(x_i)|^{p+1}\,|x-x_i|}} \tag{80}$$

or equivalently,

$$\sqrt[p+1]{\Delta^{(p)}(x)} = |\pi(x)| \sqrt[p+1]{\sum_{i=0}^{n} \frac{1}{p!\,|\pi'(x_i)|^{p+1}\,|x - x_i|}} \tag{81}$$

We note that this expression is a homogeneous function of $\pi(x)$ of degree 0.

We conjecture that the variations of the above criterion, as $p \to \infty$, are dominated by those of the factor $|\pi(x)|$. Hence, in this limit, the optimal distribution of interpolation points should approach the Chebyshev distribution.

5.5 Overall bound on the approximation error

The quantity $\epsilon\Delta^{(p)}(x)$ is an absolute bound on the error committed in the computation of the generalized Hermitian interpolant based on function and derivative values in presence of uncertainties on the derivatives of highest-order, p, only, when these are uniformly bounded by ϵ :

$$\forall x \in [-1,1]\,,\ \left|\delta \mathsf{H}_{n,p}(x)\right| = \left|\bar{\mathsf{H}}_{n,p}(x) - \mathsf{H}_{n,p}(x)\right| \le \epsilon\Delta^{(p)}(x) \tag{82}$$

where $\bar{\mathsf{H}}_{n,p}(x)$ represents the actually computed approximation.

On the other hand, the interpolation error is the difference between the actual function value, $f(x)$, and the "true" interpolant, $\mathsf{H}_{n,p}(x)$, that could be computed if all function and derivative information were known. The interpolation error satisfies :

$$\forall x \in [-1,1]\,,\ \left|f(x) - \mathsf{H}_{n,p}(x)\right| = \left|\pi(x)^{p+1} \frac{f^{([(p+1)(n+1)])}(\xi)}{[(p+1)(n+1)]!}\right| \le \mu_{n,p}\,|\pi(x)|^{p+1} \tag{83}$$

where one has let :

$$\mu_{n,p} = \max_{x\in[-1,1]} \left|\frac{f^{([(p+1)(n+1)])}(x)}{[(p+1)(n+1)]!}\right| \tag{84}$$

Consequently, we have :

$$\boxed{\forall x \in [-1,1]\,,\ \left|f(x) - \bar{\mathsf{H}}_{n,p}(x)\right| \le \mu_{n,p}\,|\pi(x)|^{p+1} + \epsilon\Delta^{(p)}(x)} \tag{85}$$

Now, examining the precise expression for $\Delta^{(p)}(x)$, that is (80), we see that the ratio of the second term to the first on the right of the above inequality is equal to

$$\frac{\epsilon}{\mu_{n,p}} \sum_{i=0}^{n} \frac{1}{p!\,|\pi'(x_i)|^{p+1}\,|x - x_i|} \tag{86}$$

For given n and p, this expression is unbounded in x. Thus, the (bound on) the error is inevitably degraded in order of magnitude due in presence of uncertainties.

However, the actual dilema of interest is somewhat different. It is the following : given the values $\{y_i, y_i', ..., y_i^{(p-1)}\}$ $(0 \le i \le n)$, and correspondingly, approximations of the higher derivative $\{y_i^{(p)}\}$, which of the following two interpolants is (guaranteed to be) more accurate :

1. the Hermitian interpolant of the sole exact values : $\{y_i, y_i', ..., y_i^{(p-1)}\}$ $(0 \le i \le n)$, or
2. the Hermitian interpolant of the entire data set?

The first interpolant differs from $f(x)$ by the sole interpolation error, $\mu_{n,p-1}\,|\pi(x)|^p$. The second interpolant is associated with a higher-order interpolation error, $\mu_{n,p}\,|\pi(x)|^{p+1}$, but is subject to the uncertainty term, $\epsilon\Delta^{(p)}(x)$, which is dominant, as we have just seen. Thus, the decision of including derivatives or not, should be guided by the ratio of the uncertainty term, $\epsilon\Delta^{(p)}(x)$, to the lower interpolation error, $\mu_{n,p-1}\,|\pi(x)|^p$. This ratio is equal to :

$$\frac{\epsilon}{\mu_{n,p-1}}\,|\pi(x)|\sum_{i=0}^{n}\frac{1}{p!\,|\pi'(x_i)|^{p+1}\,|x-x_i|} \tag{87}$$

and it admits the bound :

$$\frac{\epsilon B_{n,p}}{\mu_{n,p-1}} \tag{88}$$

where the bound,

$$B_{n,p}=\max_{x\in[-1,1]}|\pi(x)|\sum_{i=0}^{n}\frac{1}{p!\,|\pi'(x_i)|^{p+1}\,|x-x_i|} \tag{89}$$

exists since in the above, the function over which the max applies is piecewise polynomial for fixed n and p.

Hermitian interpolation is definitely preferable whenever the expression in (88) is less than 1. This criterion permits us to identify trends as ϵ, n and p vary, but is not very practical in general since the factors ϵ and $\mu_{n,p-1}$ are problem-dependent, and out of control. The variation with n of the bound $B_{n,p}$ has been plotted on Figure 1 for $p=1$, 2 and 3. Visibly, the bound $B_{n,p}$ can be large unless p and n are small. Therefore, unsurprisingly, unless n and p, as well as the uncertainty level ϵ, are small enough, the criterion in (88) is larger than 1, and the interpolant of the sole exactly-known values is likely to be the more accurate.

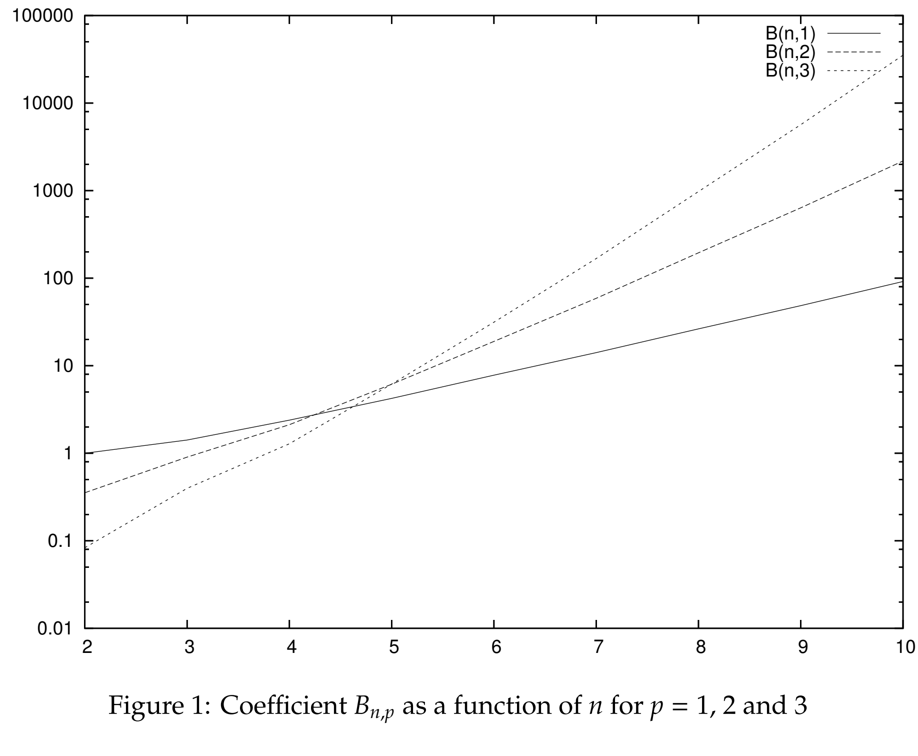

Figure 1: Coefficient $B_{n,p}$ as a function of n for $p=1$, 2 and 3

To appreciate this in a practical case, we have considered the case of the interpolation of the function

$$f(x)=f_\lambda(x)=\frac{1}{1+\lambda x^2} \tag{90}$$

over the interval [-1,1] for $p=0$ (Lagrange interpolation) and $p=1$ (Hermitian interpolation). This smooth function is bounded by 1, and its maximum derivative increases with λ. For $\lambda=64/27$, this maximum is equal to 1. For $\lambda=256/27$, this maximum is equal to 2.

In a first experiment (Figures 2 and 3), $\lambda = 64/27$, and $n = 5$. The Lagrange interpolant is fairly inaccurate, mostly near the endpoints. Thus the error distribution indicates that the approximate Hermitian interpolant is preferable even for a fairly-high level of uncertainty on the derivatives (20 % is acceptable).

In the second experiment (Figures 4 and 5), the interpolated function is the same, but the number n is doubled ($n = 10$). Consequently, the Lagrange interpolant of the sole exact function values is very accurate. The approximate Hermitian interpolant can only surpass it, if the level of uncertainty on the derivatives is small (less than 5 %).

Lastly, with the same number of interpolation points ($n = 10$), we have considered the case of a function with larger derivatives ($\lambda = 256/27$). As a result (see Figures 6 and 7), the accuracy of the Lagrange interpolation has been severely degraded. Then again, the approximate Hermitian interpolation is found superior for higher levels of uncertainty in the derivatives (the switch is between 20 and 50 %).

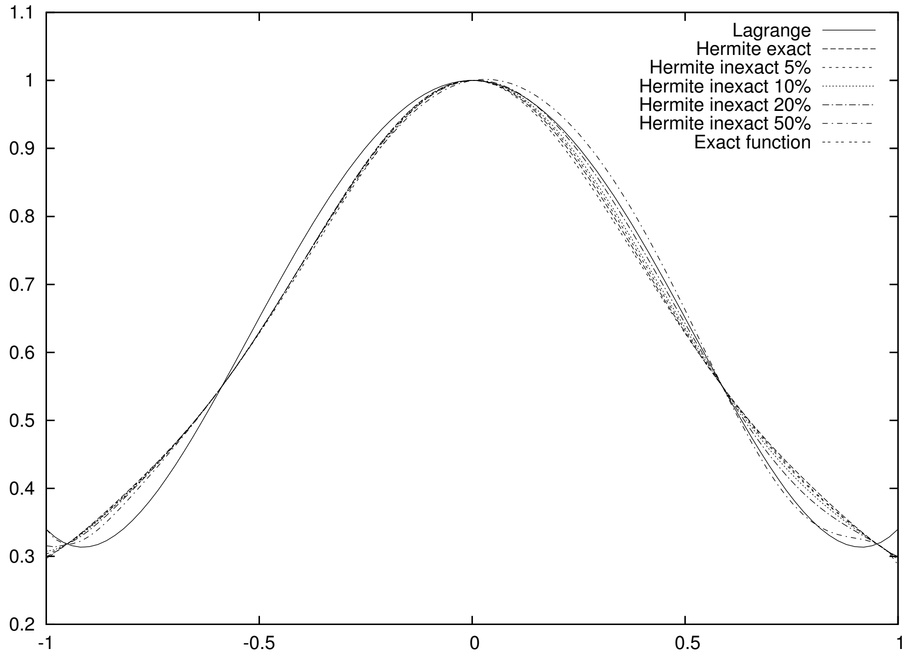

Figure 2: Case $\lambda = 64/27$ ($\max_x \left|f_\lambda(x)\right| = \max_x \left|f'_\lambda(x)\right| = 1$); function $f_\lambda(x)$ and various interpolation polynomials ($n = 5$)

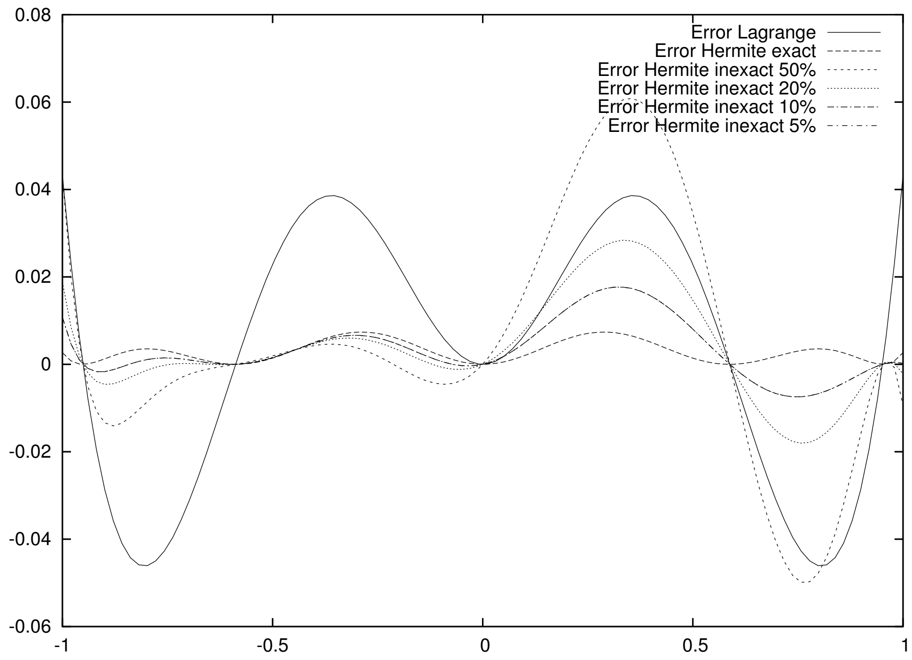

Figure 3: Case $\lambda = 64/27$ ($\max_x \left|f_\lambda(x)\right| = \max_x \left|f'_\lambda(x)\right| = 1$); error distribution associated with the various interpolation polynomials ($n = 5$)

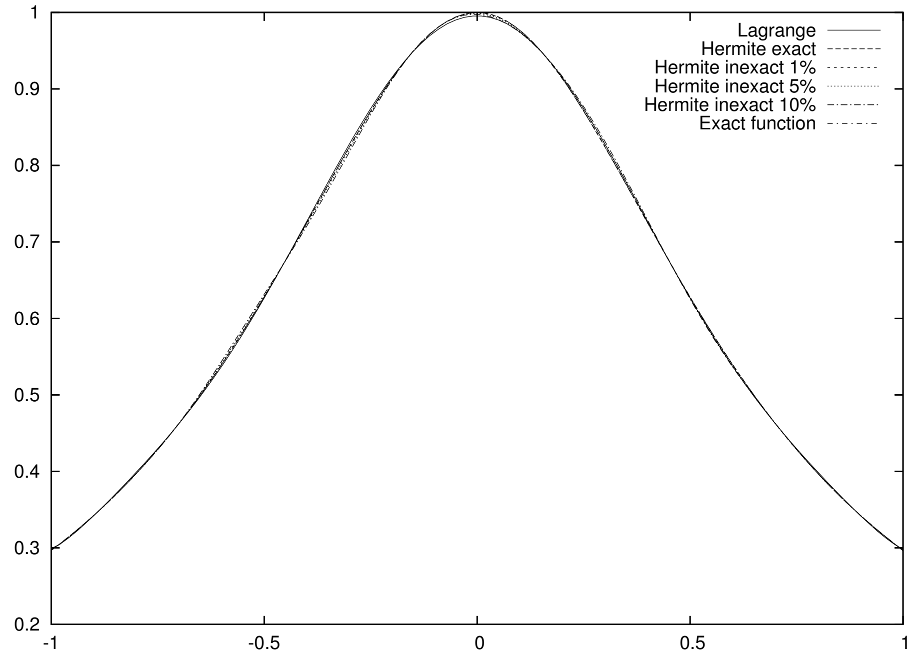

Figure 4: Case $\lambda = 64/27$ ($\max_x \left|f_\lambda(x)\right| = \max_x \left|f'_\lambda(x)\right| = 1$); function $f_\lambda(x)$ and various interpolation polynomials ($n = 10$)

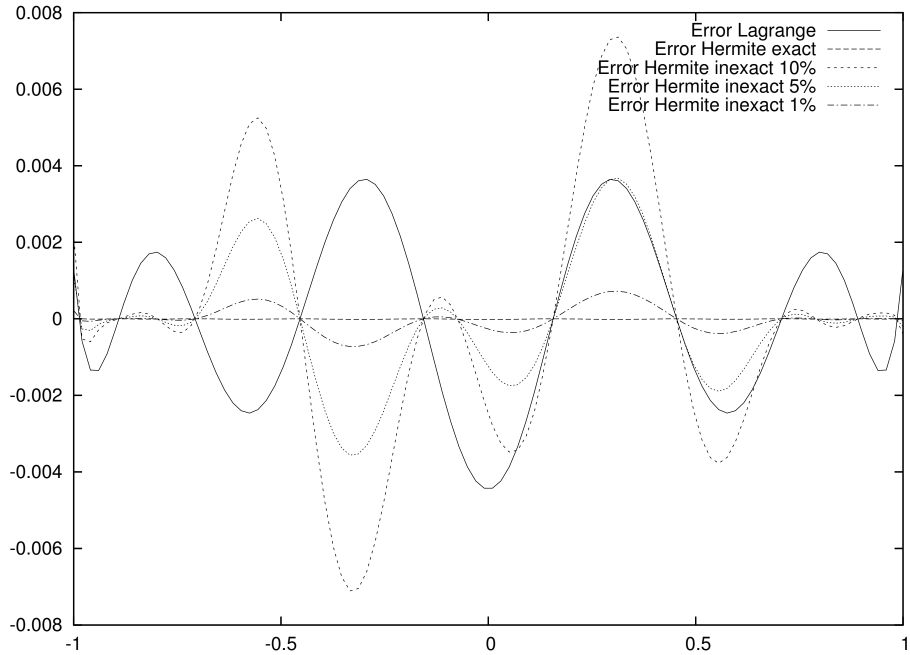

Figure 5: Case $\lambda = 64/27$ ($\max_x \left|f_\lambda(x)\right| = \max_x \left|f'_\lambda(x)\right| = 1$); error distribution associated with the various interpolation polynomials ($n = 10$)

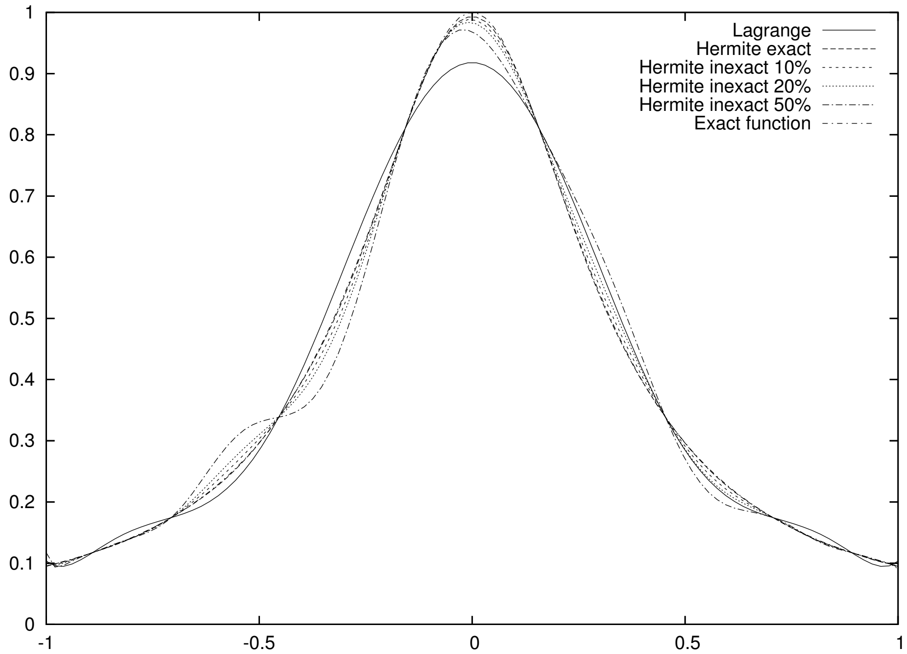

Figure 6: Case $\lambda = 256/27$ ($\max_x \left|f_\lambda(x)\right| = 1$; $\max_x \left|f'_\lambda(x)\right| = 2$); function $f_\lambda(x)$ and various interpolation polynomials ($n = 10$)

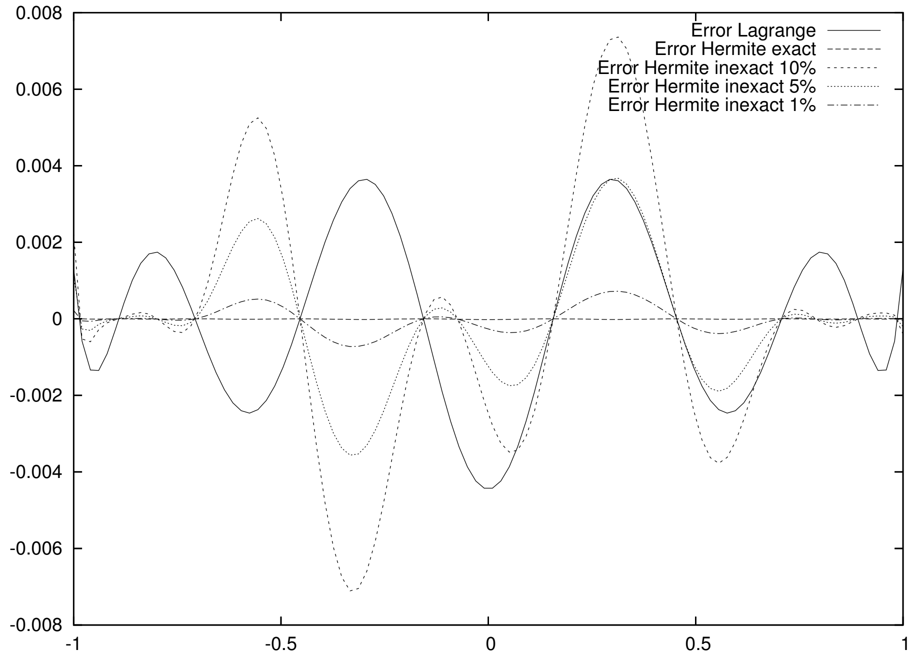

Figure 7: Case $\lambda = 256/27$ ($\max_x \left|f_\lambda(x)\right| = 1$; $\max_x \left|f'_\lambda(x)\right| = 2$); error distribution associated with the various interpolation polynomials ($n = 10$)

6 Conclusions

Recalling that the Chebyshev distribution of interpolation points is optimal w.r.t. the minimization of the (known bound on the) interpolation error, we have proposed an alternate criterion to be subject to the min-max optimization to minimize instead the sensitivity of the Hermitian interpolant of function values and derivatives to uncertainties in the derivatives only. We have found by analytical developments and numerical experiments that the Chebyshev distribution is close to be optimum w.r.t. this new criterion also, thus giving the stability of the corresponding approximation a larger sense.

We have also considered the generalized Hermitian interpolation problem in which the derivatives up to some order p ($p > 1$) are fitted. For this problem we have derived the existence and uniqueness result, as well as the expression of the interpolation error, and also the definition that one could use for the criterion to be subject to the min-max optimization to reduce the sensitivity of the interpolant to uncertainties in the derivatives of highest-most order. We conjectured from the derived expression that the corresponding optimal distribution of interpolation points converges to the Chebyshev distribution as $p \to \infty$.

Lastly, we have made actual interpolation experiments in cases of a function bounded by 1, whose derivative is either bounded by 1 or 2. These experiments have confirmed that the approximate Hermitian interpolant was superior to the Lagrange interpolant of the sole exact function values, when the uncertainty on the derivatives is below a certain critical value which decreases when n is increased.

A Case of a single interpolation point ($n = 0$)

According to the general notation, when a single interpolation point is considered $n = 0$, $\alpha = 1$ and $m = 0$, and the three distributions are identical and correspond to :

$$x_0^u = x_0^* = \bar{x}_0 = \xi_0 = 0 \tag{91}$$

so that :

$$\Delta^u = \Delta^* = \bar{\Delta} = \max_{x\in[0,1]} \Delta(x) \tag{92}$$

where

$$\Delta(x) = \pi^2(x)\frac{1}{{\pi'_0}^2 x} = x \tag{93}$$

since $\pi(x) = x$. This gives :

$$\Delta^u = \Delta^* = \bar{\Delta} = 1 \tag{94}$$

B Case of two interpolation points ($n = 1$)

Here $n = 1$, $\alpha = 0$ and $m = 1$, and we have two symmetrical interpolation points located at $\pm\xi_1$.

For all three distributions, the maximum δ_0 of $\Delta(x)$ over $[0, \xi_1]$ is given by (55), and the maximum δ_1 of $\Delta(x)$ over $[\xi_1, 1]$ by (57), and :

$$\max_{x\in[0,1]} \Delta(x) = \max(\delta_0, \delta_1) \tag{95}$$

Since $\pi(x) = x^2 - \xi_1^2$, $\pi_1' = 2\xi_1$ and (55) yields :

$$\delta_0 = 2\xi_1^4 \frac{1}{\xi_1 {\pi_1'}^2} = \frac{\xi_1}{2} \tag{96}$$

whereas :

$$\delta_1 = \left(1 - \xi_1^2\right)^2 \times 2 \times \frac{1}{{\pi_1'}^2 \left(1 - \xi_1^2\right)} = \frac{1 - \xi_1^2}{2\xi_1^2} \tag{97}$$

Hence, for the uniform distribution, $\xi_1 = \xi_1^u = 1$, $\delta_0 = \frac{1}{2}$, $\delta_1 = 0$, and :

$$\Delta^u = \tfrac{1}{2} \tag{98}$$

For the Chebyshev distribution, $\xi_1 = \xi_1^* = \frac{1}{\sqrt{2}}$, $\delta_0 = \frac{1}{2\sqrt{2}}$ and $\delta_1 = \frac{1}{2}$ and :

$$\Delta^* = \tfrac{1}{2} \tag{99}$$

The optimal distribution is achieved when

$$\delta_0 = \delta_1 \Longleftrightarrow \frac{\xi_1}{2} = \frac{1 - \xi_1^2}{2\xi_1^2} \Longleftrightarrow \xi_1^3 + \xi_1^2 = 1 \tag{100}$$

Letting

$$\xi_1 = \frac{2\cosh t - 1}{3} \tag{101}$$

yields :

$$\xi_1^2 = \frac{4\cosh^2 t - 4\cosh t + 1}{9} \qquad \xi_1^3 = \frac{8\cosh^3 t - 12\cosh^2 t + 6\cosh t - 1}{27} \tag{102}$$

and :

$$\xi_1^2 + \xi_1^3 = \frac{8\cosh^3 t - 6\cosh t + 2}{27} = \frac{2\cosh(3t) + 2}{27} = 1 \Longrightarrow \cosh(3t) = \frac{25}{2} \tag{103}$$

From this we get :

$$t \doteq 1.0724 \qquad \bar{\xi}_1 \doteq 0.7549 \qquad \bar{\Delta} = \frac{\bar{\xi}_1}{2} \doteq 0.3774 \tag{104}$$

C Case of three interpolation points ($n = 2$)

Here $n = 2$, $\alpha = 1$ and $m = 1$, and the three interpolation points are located at 0 and $\pm\xi_1$. Since $n + 1$ is odd, (55) does not hold, but (57) does. One has :

$$\pi(x) = x(x^2 - \xi_1^2) \qquad \pi'(x) = 3x^2 - \xi_1^2 \qquad \pi'_0 = -\xi_1^2 \qquad \pi'_1 = 2\xi_1^2 \tag{105}$$

Over the first interval, $x \in [0, \xi_1]$, (48) gives :

$$\Delta(x) = \frac{x^2(x^2 - \xi_1^2)^2}{\xi_1^4}\left[\frac{1}{x} + \frac{1}{4}\frac{2\xi_1}{\xi_1^2 - x^2}\right] = \frac{x(\xi_1^2 - x^2)}{2\xi_1^4}\left[2(\xi_1^2 - x^2) + \xi_1 x\right] \tag{106}$$

Letting

$$\delta = \frac{2\Delta(x)}{\xi_1} \qquad s = \frac{x}{\xi_1} \tag{107}$$

gives :

$$\delta = s(1 - s^2)(2 - 2s^2 + s) \tag{108}$$

The graph of $\delta(s)$ as s varies from 0 to 1 indicates that it is a unimodal function with a unique maximum at say $s = \bar{s}$, close to $\frac{1}{2}$, at which point $\delta = \bar{\delta}$, close to $\frac{3}{4}$ (see FIG. 8).

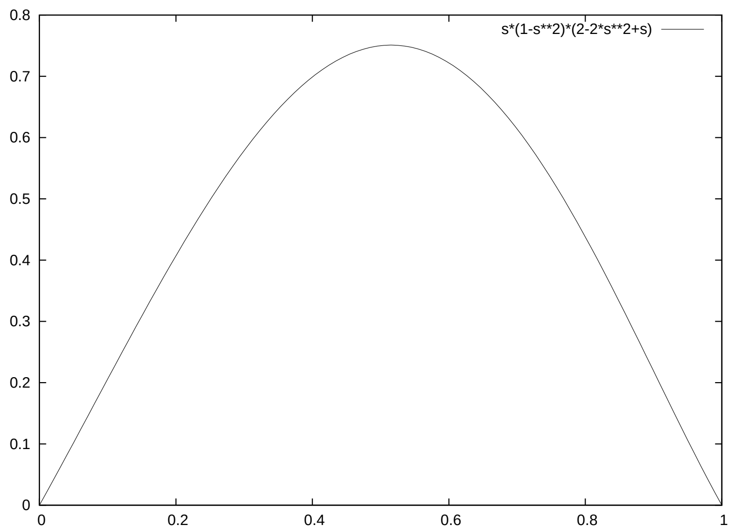

Figure 8: Function $\delta(s)$

The results of the first five Newton's iterations applied to the equation

$$\delta'(s) = 10s^4 - 4s^3 - 12s^2 + 2s + 2 = 0 \tag{109}$$

are indicated in Table 2 This iteration gives us :

$$\bar{s} \doteq 0.5155419987 \qquad \bar{\delta} \doteq 0.7509730159 \tag{110}$$

Finally, recall that :

$$\delta_0 = \max_{x \in [0, \xi_1]} \Delta(x) = \bar{\delta}\frac{\xi_1}{2} \tag{111}$$

iteration i	estimate $\bar{s}_i$	estimate $\bar{\delta}_i$
0	0.5	0.75
1	0.5156250000	0.7509729881
2	0.5155420007	0.7509730159
3	0.5155419987	0.7509730159
4	0.5155419987	0.7509730159
5	0.5155419987	0.7509730159

Table 2: Newton's iterations applied to the equation $\delta'(s) = 0$

One must now examine the complementary interval $[\xi_1, 1]$ over which the maximum of $\Delta(x)$ is given by (57) :

$$\delta_1 = \max_{x \in [\xi_1, 1]} \Delta(x) = \Delta(1) = \left(1 - \xi_1^2\right)^2 \left[\frac{1}{\pi_0'^2} + 2 \frac{1}{\pi_1'^2 \left(1 - \xi_1^2\right)} \right] = \frac{1 - \xi_1^2}{2\xi_1^4} \left[2\left(1 - \xi_1^2\right) + 1 \right] \tag{112}$$

Now, the maximum of $\Delta(x)$, when x varies from 0 to 1, is equal to the maximum of δ_0 and δ_1, that are both functions of ξ_1. But, by inspection, as ξ_1 varies from 0 to 1, δ_1 decreases from $+\infty$ to 0, whereas δ_0 increases linearly. Therefore, the maximum of the two is minimized when they are equal :

$$\delta_0 = \delta_1 \tag{113}$$

and this occurs for a unique ξ_1 hereafter denoted $\bar{\xi}_1$. Thus, $\bar{\xi}_1$ is the unique root in [0,1] of the equation :

$$\bar{\delta} \frac{\bar{\xi}_1}{2} = \frac{1 - \bar{\xi}_1^2}{2\bar{\xi}_1^4} \left[3 - 2\bar{\xi}_1^2 \right] \tag{114}$$

which can be rearranged as follows :

$$\bar{\delta} \bar{\xi}_1^5 = \left(1 - \bar{\xi}_1^2\right)\left(3 - 2\bar{\xi}_1^2\right) \tag{115}$$

The results first five Newton's iterations applied to the polynomial equation are indicated in Table 3, from which the optimal ξ_1 is obtained :

$$\bar{\xi}_1 \doteq 0.8676697403 \tag{116}$$

and the corresponding value for the min-max is :

$$\bar{\Delta} = \frac{\bar{\xi}_1}{2} \bar{\delta} \doteq 0.3258 \tag{117}$$

iteration i	estimate $\bar{\xi}_1$
0	0.85
1	0.8677214109
2	0.8676697407
3	0.8676697403
4	0.8676697403
5	0.8676697403

Table 3: Newton's iterations applied to (115) to determine $\bar{\xi}_1$

D Case of four interpolation points ($n = 3$)

D.1 Generalities

Here $n = 3$, $\alpha = 0$ and $m = 2$, and the four interpolation points are located at $\pm\xi_1$ and $\pm\xi_2$, denoted $\pm\xi$ and $\pm\eta$ ($\eta > \xi > 0$) for simplicity, and :

$$\max_{x\in[0,1]} \Delta(x) = \max(\delta_0, \delta_i, \delta_1) \tag{118}$$

where :

$$\delta_0 = \max_{x\in[0,\xi]} \Delta(x) \qquad \delta_i = \max_{x\in[\xi,\eta]} \Delta(x) \qquad \delta_1 = \max_{x\in[\eta,1]} \Delta(x) \tag{119}$$

Additionally :

$$\pi(x) = (x^2 - \xi^2)(x^2 - \eta^2) \qquad \pi'(\xi) = 2\xi(\xi^2 - \eta^2) < 0 \qquad \pi'(\eta) = 2\eta(\eta^2 - \xi^2) > 0 \tag{120}$$

Since $n + 1$ is even, δ_0 can be computed by (55) :

$$\delta_0 = \frac{2\xi^3}{\pi'(\xi)^2}\eta^4 + \frac{2\eta^3}{\pi'(\eta)^2}\xi^4 = \frac{\xi\eta(\xi^3 + \eta^3)}{2\,(\eta^2 - \xi^2)^2} \tag{121}$$

The value of δ_1 can be computed by (57) :

$$\begin{aligned}\delta_1 &= \left(1 - \xi^2\right)^2 \left(1 - \eta^2\right)^2 \left[2\frac{1}{\pi'(\xi)^2\,(1 - \xi^2)} + 2\frac{1}{\pi'(\eta)^2\,(1 - \eta^2)}\right] \\ &= \frac{\left(1 - \xi^2\right)^2 \left(1 - \eta^2\right)^2}{2\xi^2\eta^2\,(\eta^2 - \xi^2)^2} \left[\xi^2(1 - \xi^2) + \eta^2(1 - \eta^2)\right]\end{aligned} \tag{122}$$

Lastly, over the intermediate interval ($\xi \le x \le \eta$), the function $\Delta(x)$ is given by (48) with $j = m = 2$:

$$\Delta(x) = \delta(x) \qquad (\xi \le x \le \eta) \tag{123}$$

where :

$$\begin{aligned}\delta(x) &= \left(x^2 - \xi^2\right)^2 \left(x^2 - \eta^2\right)^2 \left[\frac{1}{\pi'(\xi)^2}\frac{2x}{x^2 - \xi^2} + \frac{1}{\pi'(\eta)^2}\frac{2\eta}{\eta^2 - x^2}\right] \\ &= \frac{\left(x^2 - \xi^2\right)\left(\eta^2 - x^2\right)}{2(\eta^2 - \xi^2)^2} \underbrace{\left[\frac{x\left(\eta^2 - x^2\right)}{\xi^2} + \frac{x^2 - \xi^2}{\eta}\right]}_{:=q(x)}\end{aligned} \tag{124}$$

Thus, $\delta(x)$ is a 7th-degree polynomial in x four roots of which are obvious, $\pm\xi$ and $\pm\eta$, and real. The other three are the roots of the 3rd-degree polynomial $q(x)$, above between brackets. But,

$$q'(x) = \frac{-3x^2 + \eta^2}{\xi^2} + \frac{2x}{\eta} = \frac{-3\eta x^2 + 2\xi^2 x + \eta^3}{\xi^2\eta} \tag{125}$$

Define the discriminant $d = b'^2 - ac = \xi^4 + 3\eta^4 > 0$. The roots of $q'(x)$ are thus real and given by :

$$r_{1,2} = \frac{\xi^2 \mp \sqrt{\xi^4 + 3\eta^4}}{3\eta} \tag{126}$$

Obviously $r_1 < 0$ and $r_2 > 0$. The sign of $q'(x)$ as x varies, and the variations of $q(x)$ are indicated on Table 4 in which :

$$q_1 = q(r_1) \qquad q_0 = q(0) \qquad q_2 = q(r_2) \tag{127}$$

x	$-\infty$	$\hat{\xi}_1$	r_1	0	$\hat{\xi}_2$	r_2	$\hat{\xi}_3$	$+\infty$
$q'(x)$	$-\infty$	$-$	0	$+$	$+$	0	$-$	$+\infty$
$q(x)$	$+\infty$	0	q_1	q_0	0	q_2	0	$-\infty$

Table 4: Variations of $q(x)$

Since $q'(x) > 0$ when $x \in [r_1, 0]$, $q_1 < q_0 = -\frac{\xi^2}{\eta} < 0$. Therefore, $q(x)$ admits a root $\hat{\xi}_1 < r_1$. Additionally, suppose that we had $q_2 \leq 0$. Then $q(x)$ would be uniformly non-positive for $x \geq 0$. But this is not so, since $q(\xi) = \frac{\eta^2-\xi^2}{\xi^2} > 0$. Therefore $q_2 > 0$, and $q(x)$ admits two additional real roots, $\hat{\xi}_2 \in [0, r_2]$ and $\hat{\xi}_3 > r_2$.

Consequently all seven roots of $\delta(x)$ are real . Three of them are negative ($\hat{\xi}_1$, $-\xi$ and $-\eta$), and the other four positive (ξ, η, $\hat{\xi}_2$ and $\hat{\xi}_3$). This pattern is depicted on Fig. 9, where the position of each root w.r.t. the other six will now established precisely.

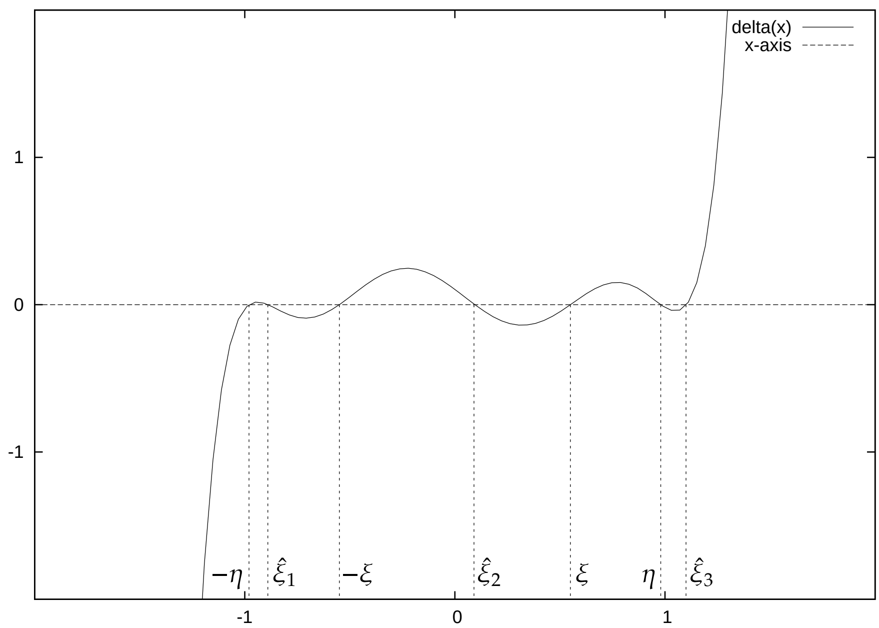

Figure 9: Graph of the 7th-degree polynomial $\delta(x)$, here drawn for $\xi = 0.55$ and $\eta = 0.98$ as a typical example

Let us show that the positive roots are ordered as follows :

$$0 \leq \hat{\xi}_2 \leq \xi \leq \eta \leq \hat{\xi}_3 \tag{128}$$

as taken for granted in Fig. 9.

By definition of the symbols, ξ, which is positive and less than η, is one of the first three positive roots of $\delta(x)$. But,

$$\delta'(\xi) = \frac{(2\xi)\left(\eta^2 - \xi^2\right)}{2(\eta^2 - \xi^2)^2}\left[\frac{\xi\left(\eta^2 - \xi^2\right)}{\xi^2} + 0\right] = 1 > 0 \tag{129}$$

and this excludes the possibility for ξ to be the first or the third positive root at which the derivative is negative. Therefore ξ is the second positive root of $\delta(x)$. Similarly,

$$\delta'(\eta) = \frac{(-2\eta)\left(\eta^2 - \xi^2\right)}{2(\eta^2 - \xi^2)^2}\left[\frac{\eta^2 - \xi^2}{\xi^2} + 0\right] = -1 < 0 \tag{130}$$

Therefore, η is the third positive root of $\delta(x)$, and this concludes the proof of the claim made above concerning the ordering of the positive roots of $\delta(x)$. □

Consequently, the function $\Delta(x) = \delta(x)$ over $[\xi, \eta]$, is unimodal and concave over this interval. It admits a unique maximum achieved at a unique point $x = \zeta$, and

$$\delta_i = \delta(\zeta) \tag{131}$$

D.2 Numerical treatment.

The numerical optimization of (ξ, η) has been performed in two steps :

Step 1: Coarse determination

1. The parameter ξ is discretized in [0,1].
2. The parameter η is discretized in $[\xi, 1]$.
3. Given ξ and η, δ_0 and δ_1 are computed.
4. The variable x is discretized, $\delta(x)$ tabulated and δ_i identified.
5. The maximum $\max(\delta_0, \delta_i, \delta_1)$ is stored.

At completion of the above nested loops, the min-max is identified, coarsely, as well as $\bar{\xi}$ and $\bar{\eta}$. One verifies that the optimum is realized when :

$$\delta_0 = \delta_i = \delta_1 \tag{132}$$

Step 2: Fine determination This step only differs from Step 1 in the first two items that are carried out knowing that we are seeking for a solution of (132), by making less but finer discretizations as follows:

1. The parameter ξ is finely discretized in [0,1].
2. The parameter η is equally-finely discretized in $[\xi, 1]$, and an interval containing the solution η of the equation $\delta_0 = \delta_1$ is identified, and a linear interpolation is used to determine η. (We show next that this equation admits a unique positive solution.)

As a result of the above procedure, we have found the following approximate values :

$$\bar{\xi} \doteq 0.351 \qquad \bar{\eta} \doteq 0.926 \tag{133}$$

yielding :

$$\bar{\Delta} \doteq 0.252 \tag{134}$$

whereas an independent program has given:

$$\Delta^* \doteq 0.299 \qquad \Delta^u \doteq 0.439 \tag{135}$$

To illustrate these results, the 3D plot of the function

$$z(\xi,\eta) = \max_{x\in[0,1]} \Delta(x;\xi,\eta) \tag{136}$$

is given in Fig. 10, and its contour plot in Fig. 11.

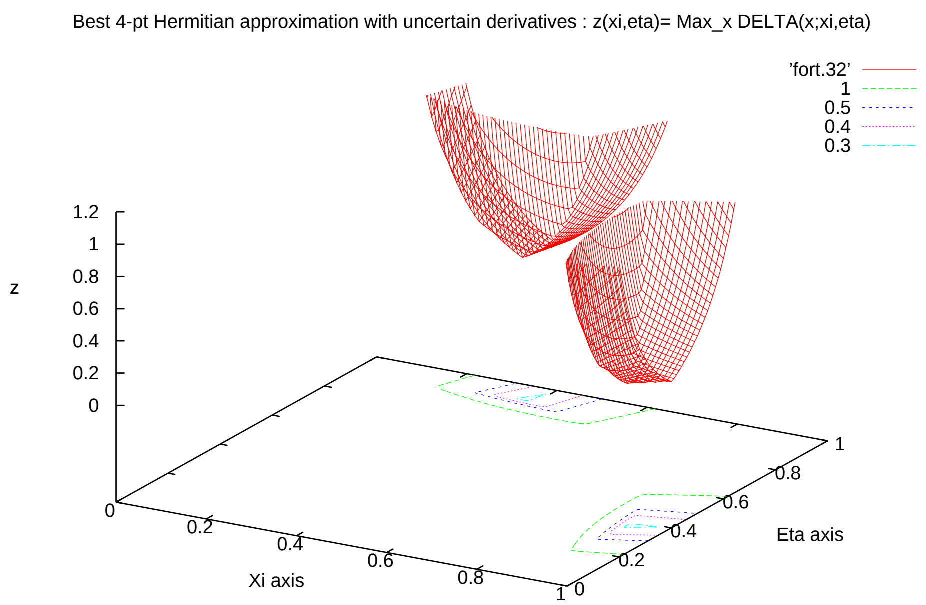

Figure 10: 3D plot of function $z(\xi,\eta)$ of (136) for $n+1=4$

As mentioned above, we conclude this section by proving a uniqueness result.

D.3 Existence and uniqueness of a solution $\eta^* > 0$ to the equation $\delta_0 = \delta_1$ for fixed $\xi \in]0,1[$

Existence. The equation $\delta_0 = \delta_1$ is equivalent to the folllowing polynomial equation :

$$f(\xi,\eta) = g(\xi,\eta) \tag{137}$$

where :

$$\begin{cases} f(\xi,\eta) = \xi^3\eta^3(\xi^3+\eta^3) \\ g(\xi,\eta) = (1-\xi^2)(1-\eta^2)\left[\xi^2(1-\xi^2)+\eta^2(1-\eta^2)\right] \end{cases} \tag{138}$$

For fixed $\xi \in]0,1[$, with the exception of the unique solution of the equation $\xi^2+\xi^3=1$, namely $\xi \doteq 0.7549$, the equation $f=g$ is a 6th-degree polynomial equation in η whose coefficients are themselves 6th-degree polynomials in ξ. Additionally, the equation is symmetric in ξ and η.

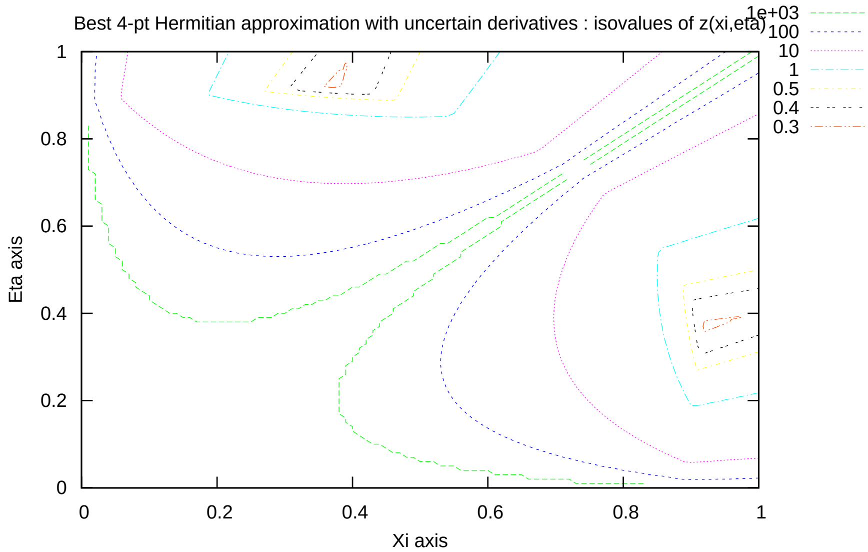

Figure 11: Contour plot of function $z(\xi, \eta)$ of (136) for $n + 1 = 4$

Then define :

$$h(\xi, \eta) = f(\xi, \eta) - g(\xi, \eta) \tag{139}$$

and again for $0 < \xi < 1$, observe that :

$$\begin{cases} h(\xi, 0) = -\xi^2(1 - \xi^2) < 0 \\ h(\xi, \xi) = 2\xi^9 - 2\xi^2(1 - \xi^2)^3 = 2\xi^2 \left[\xi^7 - (1 - \xi^2)^3\right] \\ h(\xi, 1) = \xi^3(\xi^3 + 1) > 0 \end{cases} \tag{140}$$

Note that $h(\xi, \xi) = 0$ uniquely for $\xi = 0$ or $\xi^* \doteq 0.72533$, and that $h(\xi, \xi) > 0$ iff $\xi > \xi^*$.

Since $h(\xi, 0)\, h(\xi, 1) < 0$, the equation $f = g$, or $h = 0$, admits at least one real solution in]0,1[. Let $\eta^*(\xi)$ denote this solution in case it is unique, and the smallest one otherwise. □

Uniqueness. For $\xi = 0$, the equation reduces to :

$$0 = \eta^2(1 - \eta^2)^2 = \eta^2(1 - \eta)^2(1 + \eta)^2 \tag{141}$$

and admits 3 double roots : 0 and ±1.

Recall that a classical theorem : if the coefficients of a polynomial equation in η are analytic (e.g. polynomial) functions of a parameter ξ, and if, for $\xi = \xi_0$, a root η_0 is of multiplicity $\nu \geq 1$, then in the neighborhood of $\xi = \xi_0$, a number ν of roots can be expressed as independent Taylor's series expansions of $(\xi - \xi_0)^{\frac{1}{\nu}}$ with leading term η_0.

However, let us show that there is no real branch originating from the double root $\eta_0 = 0$. For this, suppose otherwise that real couples (ξ, η) satisfying (137) exist in any, arbitrarily small, neighborhood of the origin. By symmetry, it is not restrictive to suppose that $0 < \xi \leq \eta$. Then, let us determine the orders of magnitude of various terms using the assumption that both ξ and η are infinitely small :

$$\begin{aligned}
\xi^3+\eta^3 &: \eta^3 \qquad (\text{since } \xi \leq \eta)\\
f &: \xi^3\eta^6\\
1-\xi^2 &: 1\\
1-\eta^2 &: 1\\
g &: \xi^2+\eta^2\,,\ \text{that is} : \eta^2\\
f/g &: \xi^3\eta^4
\end{aligned}$$

Hence, f would be infinitely smaller than g, and this would be in contradiction with the assumption made. Therefore, there is no real branch of solutions originating from the origin.

Let us now examine the situation about the double root $\eta_0 = 1$[1]. In the complex plane extending the real axis for η, two, possibly identical, branches emanate from the point $\eta_0 = 1$ permitting to follow by continuity, as ξ varies, two roots that can be expressed in Taylor's series of $\sqrt{\xi}$. One of these two branches at least remains real in a neighborhood of $\eta_0 = 1$, since otherwise the equation $f = g$ would locally have no real root at all, and this would be in contradiction with the previously established existence result. Hence a real branch of solutions originate from the point (0,1) in the (ξ, η)-plane; in other words, by continuity we can let $\eta^*(0) = 1$. Then we have the following :

Lemma 2
If $\eta^*(\xi) \geq \frac{1}{\sqrt{2}}$, $\eta^*(\xi)$ is the unique positive root of (137).

Proof : The parameter ξ being fixed, for $0 < \eta < \eta^*(\xi)$, $f \neq g$, since $\eta^*(\xi)$ is the smallest positive root of the equation $f = g$. For $\eta = \eta^*(\xi)$, $f = g$. But, as η increases from $\eta^*(\xi)$ on, the term $\eta^2(1-\eta^2)$ decreases since $\eta^2 > \frac{1}{2}$, and so does g, whereas f increases. Hence, f and g diverge and are never equal again. Therefore, $\eta^*(\xi)$ is the unique solution. □

Hence, in the (ξ, η)-plane, the point (0,1) is the origin of a unique branch of solutions, of analytical equation :

$$\eta = \eta^*(\xi) \tag{142}$$

at least so long as $\eta^*(\xi) \geq \frac{1}{\sqrt{2}}$.

A simple computer program was made to identify a lower and an upper bound on $\eta^*(\xi)$ for fixed $\xi \in]0, \xi^*[$ by simple discretization and test of the sign of h, knowing that $h < 0$ for $\eta < \eta^*(\xi)$, and inversely, $h > 0$ for $\eta > \eta^*(\xi)$. The corresponding result is indicated in Fig. 12. Clearly, for $0 < \xi < \xi^*$,

$$\eta^*(\xi) > \xi^* > \frac{1}{\sqrt{2}} \tag{143}$$

Therefore, the solution $\eta^*(\xi)$ is unique, at least for $\xi \in]0, \xi^*[$. The corresponding branch of solutions is completed by the symmetrical portion connecting the point (ξ^*, ξ^*) with (1,0). This new portion of the branch is also made of unique solutions, because of the following : assuming otherwise would imply that one point of this portion of the branch ($\xi^* < \xi < 1$) would correspond to a bifurcation of solutions, and by symmetry, a similar bifurcation would also exist in the first portion of the branch ($0 < \xi < \xi^*$) and this is not possible, since there, the solution has been proved to be unique. □

Lastly, remark that we have made throughout the hypothesis that $\xi^3 + \xi^2 \neq 1$. We now verify that this is indeed the case when $\xi \in [0, \xi^*]$ for which we have developed our argumentation.

[1]By symmetry, the situation about the double root $\eta_0 = -1$ is the same.

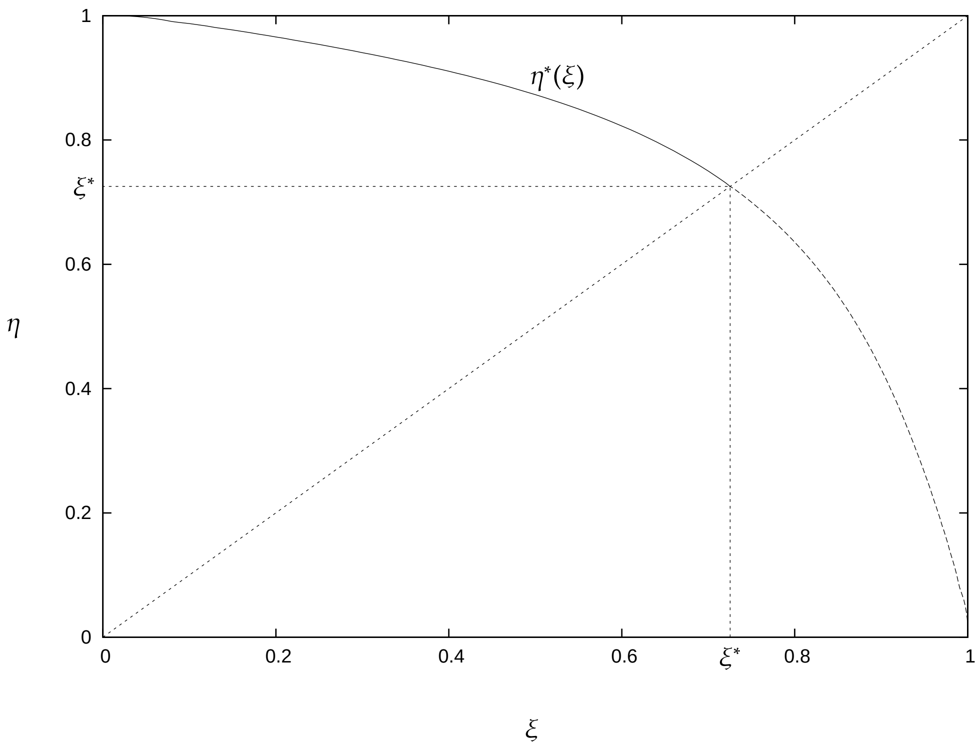

Figure 12: The root $\eta^*(\xi)$ identified numerically

E Case of five interpolation points ($n = 4$)

E.1 Generalities

Here $n = 4$, $\alpha = 1$ and $m = 2$, and the five interpolation points are located at 0, $\pm\xi_1$ and $\pm\xi_2$, denoted $\pm\xi$ and $\pm\eta$ ($\eta > \xi > 0$) for simplicity, and :

$$\max_{x\in[0,1]} \Delta(x) = \max(\delta_0, \delta_i, \delta_1) \tag{144}$$

where :

$$\delta_0 = \max_{x\in[0,\xi]} \Delta(x) \qquad \delta_i = \max_{x\in[\xi,\eta]} \Delta(x) \qquad \delta_1 = \max_{x\in[\eta,1]} \Delta(x) \tag{145}$$

Additionally :

$$\pi(x) = x(x^2-\xi^2)(x^2-\eta^2) \quad \pi'(0) = \xi^2\eta^2 \quad \pi'(\xi) = 2\xi^2(\xi^2-\eta^2) < 0 \quad \pi'(\eta) = 2\eta^2(\eta^2-\xi^2) > 0 \tag{146}$$

E.2 Analysis of $\Delta(x)$ over the first interval : $x \in [0, \xi]$

Since $n+1$ is odd, δ_0 cannot be computed by (55). Instead we apply the general formula for $\Delta(x)$, that is, (48), with $j = 1$:

$$\begin{aligned}
\Delta(x) = \delta^0(x) &= \pi^2(x)\left[\frac{1}{\pi_0'^2}\frac{1}{x} + \sum_{k=1}^{2}\frac{1}{\pi_k'^2}\frac{2\xi_k}{\xi_k^2-x^2}\right] \\
&= x^2(x^2-\xi^2)^2(x^2-\eta^2)^2\left[\frac{1}{\xi^4\eta^4}\frac{1}{x} + \frac{1}{4\xi^4(\xi^2-\eta^2)^2}\frac{2\xi}{\xi^2-x^2} + \frac{1}{4\eta^4(\eta^2-\xi^2)^2}\frac{2\eta}{\eta^2-x^2}\right] \\
&= \frac{x(\xi^2-x^2)(\eta^2-x^2)}{2\xi^4\eta^4(\eta^2-\xi^2)^2}\,P(x)
\end{aligned} \tag{147}$$

where $P(x)$ is the following 4th-degree polynomial :

$$P(x) = 2(\eta^2-\xi^2)^2(\xi^2-x^2)(\eta^2-x^2) + \xi\eta^4 x(\eta^2-x^2) + \eta\xi^4 x(\xi^2-x^2) \tag{148}$$

The polynomial $P(x)$ has the following characteristics :

- $P(0) = 2\xi^2\eta^2(\eta^2-\xi^2)^2 > 0$.
- $P(\pm\xi) = \pm\xi^2\eta^4(\eta^2-\xi^2)$.
- $P(\pm\eta) = \mp\eta^2\xi^4(\eta^2-\xi^2)$.
- $P(x) > 0$ at ∞.

Consequently, $P(x)$ has 4 distinct roots, $\{\sigma_i\}_{i=1,2,3,4}$, satisfying the following bounds :

$$-\eta < \sigma_1 < -\xi < \sigma_2 < 0 < \xi < \sigma_3 < \eta < \sigma_4 \tag{149}$$

The graph of $P(x)$ can easily be sketched. It is depicted in Fig. 13 drawn for $\xi = 0.50$ and $\eta = 0.85$ as an example.

The four zeroes $\{\sigma_i\}_{i=1,2,3,4}$ are distinct and all different from $\pm\xi$ or $\pm\eta$. Hence the 9th-degree polynomial $\delta^0(x)$ to which $\Delta(x)$ identifies over the interval $[0, \xi]$ admits the following 9 distinct zeroes written in increasing order :

$$-\eta\,,\ \sigma_1\,,\ -\xi\,,\ \sigma_2\,,\ 0\,,\ \xi\,,\ \sigma_3\,,\ \eta\,,\ \sigma_4\,, \tag{150}$$

and in particular, 0 and ξ are two consecutive ones. Therefore, in the interval $[0, \xi]$, $\Delta(x)$ is unimodal and concave : it first increases, achieves a maximum at say $x = \zeta_0$, and then decreases. As a result :

$$\delta_0 = \Delta(\zeta_0) \qquad (0 < \zeta_0 < \xi) \tag{151}$$

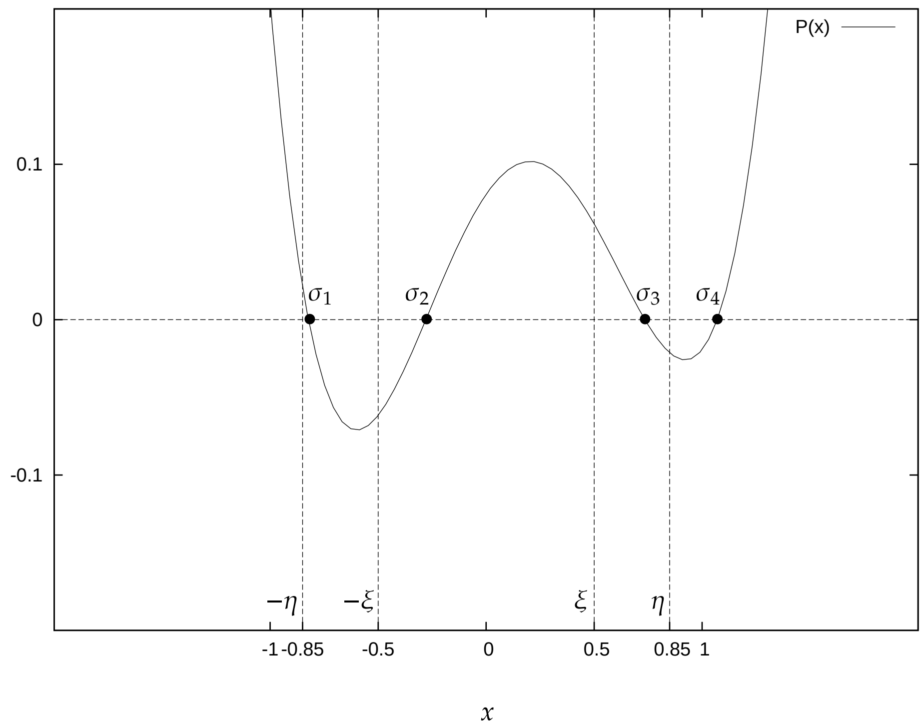

Figure 13: Sketch of the graph of the 4th-degree polynomial $P(x)$ of (148), here drawn for $\xi = 0.50$, $\eta = 0.85$

E.3 Analysis of $\Delta(x)$ over the intermediate interval : $x \in [\xi, \eta]$

Here, $\Delta(x)$ is calculated by application of (48), with $j = m = 2$:

$$\begin{aligned}
\Delta(x) = \delta^i(x) &= \pi^2(x)\left[\frac{\alpha}{\pi_0'^2}\frac{1}{x} + \frac{1}{\pi_1'^2}\frac{2x}{x^2-\xi_1^2} + \frac{1}{\pi_2'^2}\frac{2\xi_2}{\xi_2^2-x^2}\right] \\
&= x^2(x^2-\xi^2)^2(\eta^2-x^2)^2\left[\frac{1}{\xi^4\eta^4}\frac{1}{x} + \frac{1}{4\xi^4(\xi^2-\eta^2)^2}\frac{2x}{x^2-\xi^2} + \frac{1}{4\eta^4(\eta^2-\xi^2)^2}\frac{2\eta}{\eta^2-x^2}\right] \\
&= \frac{x(x^2-\xi^2)(\eta^2-x^2)}{2\xi^4\eta^4(\eta^2-\xi^2)^2}\,Q(x) \qquad (152)
\end{aligned}$$

where $Q(x)$ is the following 4th-degree polynomial :

$$Q(x) = 2(\eta^2-\xi^2)^2(x^2-\xi^2)(\eta^2-x^2) + \eta^4x^2(\eta^2-x^2) + \eta\xi^4(x^2-\xi^2) \qquad (153)$$

The polynomial $Q(x)$ is even, and has the following characteristics :

- $Q(0) = -2\xi^2\eta^2(\eta^2-\xi^2)^2 - \eta\xi^6 < 0.$
- $Q(\pm\xi) = \eta^4\xi^2(\eta^2-\xi^2) > 0.$
- $Q(\pm\eta) = \eta\xi^4(\eta^2-xi^2) > 0.$
- $Q(x) < 0$ at ∞.

Consequently, $Q(x)$ has 4 distinct roots, $\{\tau_i\}_{i=1,2,3,4}$, satisfying the following bounds :

$$\tau_1 < -\eta < -\xi < \tau_2 < 0 < \tau_3(= -\tau_2) < \xi < \eta < \tau_4(= -\tau_1) \tag{154}$$

The graph of $Q(x)$ can easily be sketched. It is depicted in Fig. 14 drawn for $\xi = 0.50$ and $\eta = 0.85$ as an example.

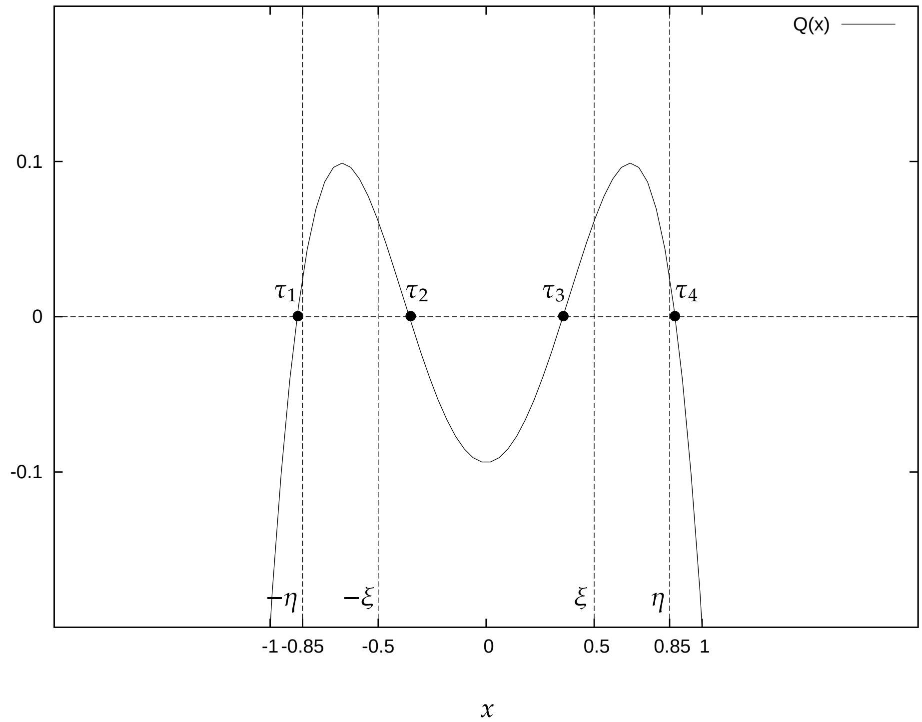

Figure 14: Sketch of the graph of the 4th-degree polynomial $Q(x)$ of (153), here drawn for $\xi = 0.50$, $\eta = 0.85$

The four zeroes $\{\tau_i\}_{i=1,2,3,4}$ are distinct and all different from $\pm\xi$ or $\pm\eta$. Hence the 9th-degree polynomial $\delta^i(x)$ to which $\Delta(x)$ identifies over the interval $[\xi, \eta]$ admits the following 9 distinct zeroes written in increasing order :

$$\tau_1\,, -\eta\,, -\xi\,, \tau_2\,, 0\,, \tau_3(= -\tau_2)\,, \xi\,, \eta\,, \tau_4(= -\tau_1)\,, \tag{155}$$

and in particular, ξ and η are two consecutive ones. Therefore, in the interval $[\xi, \eta]$, $\Delta(x)$ is unimodal and concave : it first increases, achieves a maximum at say $x = \zeta_i$, and then decreases. As a result :

$$\delta_i = \Delta(\zeta_i) \qquad (\xi < \zeta_0 < \eta) \tag{156}$$

E.4 Analysis of $\Delta(x)$ over the last interval : $x \in [\eta, 1]$

In this interval, the value of δ_1 can be computed by (57) with $\alpha = 1$ and $m = 2$:

$$\begin{aligned}\delta_1 = &= (1-\xi_1^2)^2(1-\xi_2^2)^2\left[\frac{1}{\pi_0'^2} + 2\frac{1}{\pi_1'^2\left(1-\xi_1^2\right)} + 2\frac{1}{\pi_2'^2\left(1-\xi_2^2\right)}\right] \\ &= (1-\xi^2)^2(1-\eta^2)^2\left[\frac{1}{\xi^4\eta^4} + \frac{2}{4\xi^4(\xi^2-\eta^2)^2(1-\xi^2)} + \frac{2}{4\eta^4(\eta^2-\xi^2)^2(1-\eta^2)}\right] \\ &= \frac{(1-\xi^2)(1-\eta^2)}{2\xi^4\eta^4(\eta^2-\xi^2)^2}\left[2(\eta^2-\xi^2)^2(1-\xi^2)(1-\eta^2) + \eta^4(1-\eta^2) + \xi^4(1-\xi^2)\right]\end{aligned} \tag{157}$$

E.5 Numerical treatment

The function

$$z(\xi, \eta) = \max_{x\in[0,1]} \Delta(x) = \max(\delta_0, \delta_i, \delta_1) \tag{158}$$

is calculated discretely over a fine mesh over the triangular region : $\xi \in [0, 1]$, $\eta \in [\xi, 1]$. For each couple (ξ, η), δ_0 and δ_i are calculated by a fine discretization in x and identification of the known-to-be-unique maximum of $\Delta(x)$ over the corresponding interval, that is, $[0, \xi]$ and $[\xi, \eta]$ respectively; δ_1 is calculated by the above explicit formula, (157). Lastly, $z(\xi, \eta)$ is calculated, and also assigned to $z(\eta, \xi)$. A very fine discretization was found necessary to remove wiggles in the computed results. As a result of the above numerical procedure, the 3D plot of the function $z(\xi, \eta)$ is displayed in Fig. 15, and the corresponding contours in Fig. 16.

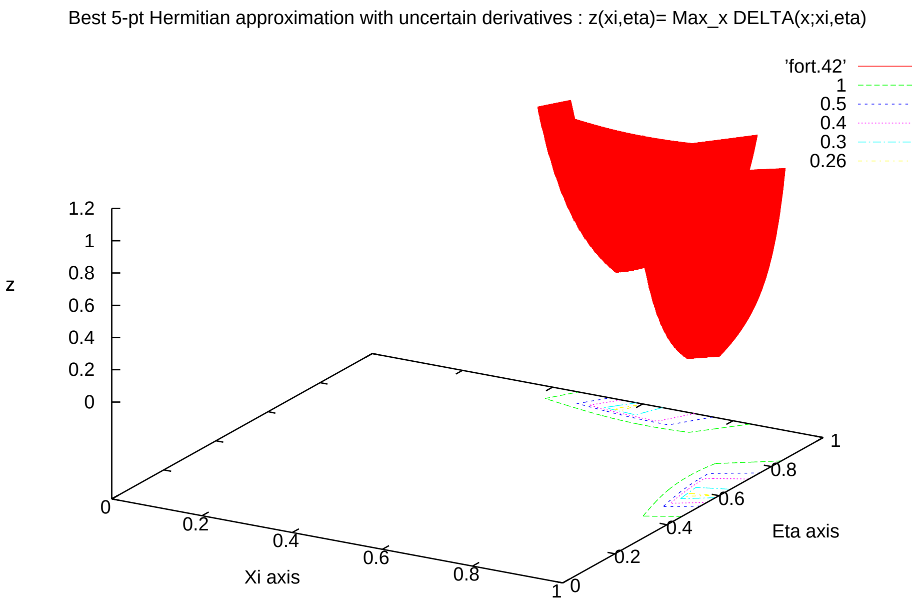

Figure 15: 3D plot of function $z(\xi, \eta)$ of (136) for $n + 1 = 5$

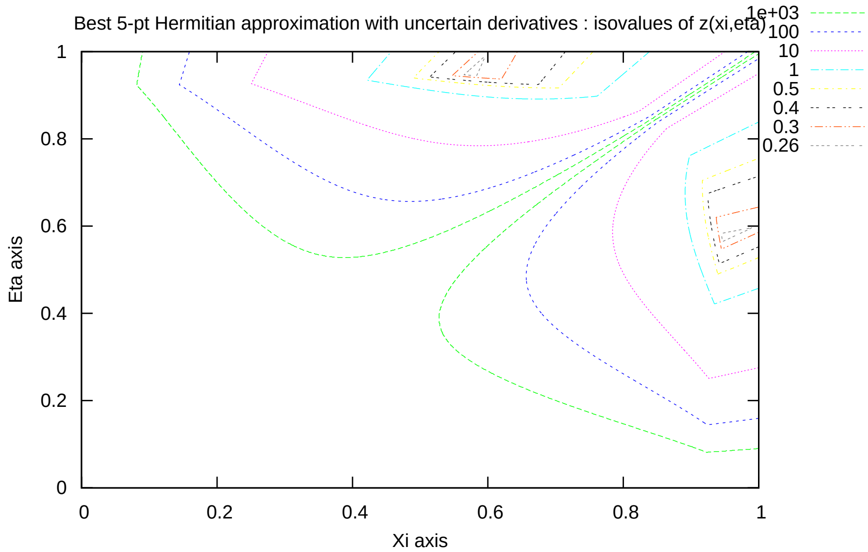

Figure 16: Contour plot of function $z(\xi,\eta)$ of (136) for $n+1=5$

It is interesting to observe in the contour plot that near the boundaries, $\xi = 1$, or $\eta = 1$, the isovalue contours are found linear.

In conclusion, we obtained the following approximations for the optimum (ξ,η) :

$$\bar{\xi} \doteq 0.571 \qquad \bar{\eta} \doteq 0.948 \tag{159}$$

for which we have verified that $\bar{\delta}_0 \doteq \bar{\delta}_i \doteq \bar{\delta}_1$, and which results in

$$\bar{\Delta} \doteq 0.249 \tag{160}$$

only slightly better than the result corresponding to the Chebyshev distribution :

$$\Delta^* \doteq 0.262 \tag{161}$$

itself better than the result corresponding to the uniform distribution :

$$\Delta^u \doteq 0.652 \tag{162}$$

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